1

10/749,450

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptau129pxo

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
* * * * * * * * * * * * *
                       Welcome to STN International
                   Web Page URLs for STN Seminar Schedule - N. America "Ask CAS" for self-help around the clock
NEWS
NEWS
                   INSPEC enhanced with 1898-1968 archive
NEWS
       3
          AUG 09
                   ADISCTI Reloaded and Enhanced
          AUG 28
NEWS
                   CA(SM)/CAplus(SM) Austrian patent law changes
          AUG 30
NEWS
                   CA/CAplus enhanced with more pre-1907 records
          SEP 11
NEWS
       6
                   CA/CAplus fields enhanced with simultaneous left and right
          SEP 21
NEWS
                   truncation
                   CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS
          SEP 25
                   CAS REGISTRY(SM) no longer includes Concord 3D coordinates CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
          SEP 25
NEWS
          SEP 25
NEWS 10
                   CEABA-VTB classification code fields reloaded with new
          SEP 28
NEWS 11
                   classification scheme
                   LOGOFF HOLD duration extended to 120 minutes
          OCT 19
NEWS 12
                   E-mail format enhanced
NEWS 13
          OCT 19
                   Option to turn off MARPAT highlighting enhancements available
NEWS 14
          OCT
               23
                   CAS Registry Number crossover limit increased to 300,000 in
          OCT 23
NEWS 15
                   multiple databases
                   The Derwent World Patents Index suite of databases on STN
NEWS 16
          OCT 23
                   has been enhanced and reloaded
                   CHEMLIST enhanced with new search and display field
          OCT 30
NEWS 17
                   JAPIO enhanced with IPC 8 features and functionality
NEWS 18
          NOV 03
                   CA/CAplus F-Term thesaurus enhanced
NEWS 19
          NOV 10
                   STN Express with Discover! free maintenance release Version
          NOV 10
NEWS 20
                   8.01c now available
                   CA/CAplus pre-1967 chemical substance index entries enhanced
          NOV 13
NEWS 21
                   with preparation role
                   CAS Registry Number crossover limit increased to 300,000 in
NEWS 22
          NOV 20
                   additional databases
                   CA/CAplus to MARPAT accession number crossover limit increased
NEWS 23
          NOV 20
                   to 50,000
                   CA/CAplus patent kind codes will be updated
          NOV 20
NEWS 24
                   CAS REGISTRY updated with new ambiguity codes
NEWS 25
          DEC 01
                NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
NEWS EXPRESS
                MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP)
                AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
                STN Operating Hours Plus Help Desk Availability
NEWS HOURS
                Welcome Banner and News Items
NEWS LOGIN
                For general information regarding STN implementation of IPC 8 X.25 communication option no longer available
NEWS IPC8
NEWS X25
```

٠. ٠.

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 04:28:36 ON 11 DEC 2006

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 3.78 3.78

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 04:39:37 ON 11 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4 DICTIONARY FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10749450.str

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR

```
Page 3
```

N<del>Hy----</del>G1

G2 G1 Me.Et.n-Pr.i-Pr.n-Bu,i-Bu,s-Bu,t-Bu G2 Ag,Cd,Co,Cu,Fe,Hg,Ni,Zn

Structure attributes must be viewed using STN Express query preparation.

=> s l1 SAMPLE SEARCH INITIATED 04:40:03 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 34809 TO ITERATE

2000 ITERATIONS 5.7% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) **SEARCH TIME: 00.00.01** 

2 ANSWERS

ONLINE \*\*COMPLETE\*\* FULL FILE PROJECTIONS: \*\*COMPLETE\*\* BATCH

PROJECTED ITERATIONS: PROJECTED ANSWERS:

685030 TO 343 TO 707330 1049

L2 2 SEA SSS SAM L1

=> search 11 ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:. ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET: full FULL SEARCH INITIATED 04:40:19 FILE 'REGISTRY' 699751 TO ITERATE FULL SCREEN SEARCH COMPLETED -

100.0% PROCESSED 699751 ITERATIONS **SEARCH TIME: 00.00.03** 

1206 ANSWERS

1206 SEA SSS FUL L1 L3

=> s triflate 791 TRIFLATE L4

 $\Rightarrow$  d 14 780-791

ANSWER 780 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN L4

14848-27-2 REGISTRY RN

Entered STN: 16 Nov 1984 ED

Methanesulfonic acid, trifluoro-, anhydride with nitrous acid (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES: CN Methanesulfonyl nitrite, trifluoro- (8CI)

OTHER NAMES:

Nitrosonium triflate CN

Trifluoromethanesulfonyl nitrite CN

C F3 N 04 S MF

```
Page 4
```

CI COM BEILSTEIN\*, BIOSIS, CA, CAPLUS, CASREACT, CHEMINFORMRX STN Files: LC (\*File contains numerically searchable property data)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE) 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

ANSWER 781 OF 791 REGISTRY COPYRIGHT 2006 ACS ON STN L4

6401-02-1 REGISTRY RN

ED

Entered STN: 16 Nov 1984 Methanesulfonic acid, trifluoro-, 2,2,3,3-tetrafluoropropyl ester (7CI, 8CI, 9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

1-Propanol, 2,2,3,3-tetrafluoro-, trifluoromethanesulfonate (8CI)

OTHER NAMES:

2,2,3,3-Tetrafluoropropan-1-yl triflate CN

2,2,3,3-Tetrafluoropropyl trifluoromethanesulfonate CN

C4 H3 F7 O3 S MF

N Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data) STN Files: LC

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

14 REFERENCES IN FILE CA (1907 TO DATE) 14 REFERENCES IN FILE CAPLUS (1907 TO DATE) 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

ANSWER 782 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN L4

6226-25-1 REGISTRY RN

Entered STN: 16 Nov 1984 ED

Methanesulfonic acid, trifluoro-, 2,2,2-trifluoroethyl ester (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

Ethanol, 2,2,2-trifluoro-, trifluoromethanesulfonate OTHER NAMES:

CN

CN

CN

2,2,2-Trifluoroethyl triflate
2,2,2-Trifluoroethyl trifluoromethanesulfonate
2,2,2-Trifluoroethyl trifluoromethylsulfonate
Trifluoromethanesulfonic acid 2,2,2-trifluoroethyl ester CN

C3 H2 F6 O3 S

```
Page 5
```

N Files: BEILSTEIN\*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM, IFICDB, IFIPAT, IFIUDB, PS, RTECS\*, SYNTHLINE, TOXCENTER, LC USPAT2, USPATFULL (\*File contains numerically searchable property data)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

164 REFERENCES IN FILE CA (1907 TO DATE) 165 REFERENCES IN FILE CAPLUS (1907 TO DATE) 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

ANSWER 783 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN L4

3857-83-8 REGISTRY RN

Entered STN: 16 Nov 1984 ED

Methanesulfonic acid, trifluoro-, 2-naphthalenyl ester (9CI) (CA INDEX CN

OTHER CA INDEX NAMES:

2-Naphthol, trifluoromethanesulfonate (8CI) CN

Methanesulfonic acid, trifluoro-, 2-naphthyl ester (7CI, 8CI) CN

β-Naphthyl triflate CN

2-((Trifluoromethanesulfonyl)oxy)naphthalene CN

CN

CN

2-Naphthalenyl triflate
2-Naphthyl triflate
2-Naphthyl trifluoromethanesulfonate CN

C11 H7 F3 O3 S MF

STN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, USPATZ, USPATFULL LC (\*File contains numerically searchable property data)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

122 REFERENCES IN FILE CA (1907 TO DATE) 122 REFERENCES IN FILE CAPLUS (1907 TO DATE) 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

ANSWER 784 OF 791 REGISTRY COPYRIGHT 2006 ACS ON STN L4

2926-30-9 REGISTRY RN

Entered STN: 16 Nov 1984 ED

Methanesulfonic acid, trifluoro-, sodium salt (8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

Sodium triflate

```
Page 6
```

```
Sodium trifluoromethanesulfonate
CN
      Sodium trifluoromethylsulfonate
CN
      Trifluoromethanesulfonic acid sodium salt
CN
      C H F3 03 S . Na
MF
      COM
CI
        N Files: ANABSTR, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT,
      STN Files:
LC
        IFIUDB, TOXCENTER, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
      (1493-13-6)
CRN
      - SO3H
  Na
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
                411 REFERENCES IN FILE CA (1907 TO DATE)
                 36 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
                412 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                  2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
      ANSWER 785 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
L4
      2926-27-4 REGISTRY
RN
      Entered STN: 16 Nov 1984
Methanesulfonic acid, trifluoro-, potassium salt (8CI, 9CI) (CA INDEX
ED
CN
      NAME)
OTHER NAMES:
      Potassium triflate
CN
      Potassium trifluoromethanesulfonate
CN
      Potassium trifluoromethylsulfonate
CN
      Trifluoromethanesulfonic acid potassium salt
CN
      32578-37-3
DR
      C H F3 03 S . K
MF
      COM
CI
        N Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL
LC
      STN Files:
           (*File contains numerically searchable property data)
      (1493-13-6)
```

CRN

```
Page 7
   C- 503H
   K
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
                 199 REFERENCES IN FILE CA (1907 TO DATE)
                 5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
199 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                    3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
      ANSWER 786 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
L4
      2923-28-6 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
      Methanesulfonic acid, trifluoro-, silver(1+) salt (8CI, 9CI) (CA INDEX
CN
      NAME)
OTHER NAMES:
      Silver (trifluoromethyl)sulfonate
CN
      Silver triflate
CN
      Silver trifluoromethanesulfonate
CN
      Silver trifluoromethanesulphonate
CN
      Silver(1+) triflate
Silver(1+) trifluoromethanesulfonate
Silver(1) triflate
CN
CN
CN
      Silver(I) trifluoromethanesulfonate
CN
      Trifluoromethanesulfonic acid silver(1+) salt
CN
      499776-24-8, 637342-85-9, 330649-44-0, 380240-12-0, 460355-11-7
DR
      C H F3 O3 S . Ag
MF
      COM
CI
         TN Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, MSDS-OHS, PROMT, TOXCENTER, USPAT2, USPATFULL
LC
      STN Files:
      (*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)
      (1493-13-6)
CRN
```

● Ag(I)

```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
               1272 REFERENCES IN FILE CA (1907 TO DATE)
               35 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1277 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
      ANSWER 787 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
L4
      2794-60-7 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
      Methanesulfonic acid, trifluoro-, barium salt (8CI, 9CI) (CA INDEX NAME)
CN
OTHER NAMES:
      Barium bis(trifluoromethanesulfonate)
CN
      Barium triflate
CN
      Barium triflate (Ba(CF3SO3)2)
CN
      Barium trifluoromethanesulfonate
CN
      C H F3 03 S . 1/2 Ba
MF
        TN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, DETHERM*, GMELIN*, IFICDB, IFIPAT, IFIUDB, USPAT2, USPATFULL

(*File contains nomerically searchable property data)
      STN Files:
LC
                          EINECS**, NDSL**, TSCA**
      Other Sources:
            (**Enter CHEMLIST File for up-to-date regulatory information)
     (1493-13-6)
CRN
     - S03H
●1/2 Ba
                  51 REFERENCES IN FILE CA (1907 TO DATE)
                  2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
52 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
      ANSWER 788 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
L4
      591-40-2 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
      Methanesulfonic acid, trifluoro-, compd. with benzenamine (1:1) (9CI) (CA
CN
      INDEX NAME)
OTHER CA INDEX NAMES:
      Benzenamine, trifluoromethanesulfonate (9CI)
      Methanesulfonic acid, trifluoro-, compd. with aniline (1:1) (8CI) Methanesulfonic acid, trifluoro-, PhNH2 salt (6CI)
CN
OTHER NAMES:
      Anilinium triflate
CN
      Anilinium trifluoromethanesulfonate
CN
      C6 H7 N . C H F3 O3 S
MF
      STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, IFICDB,
LC
         IFIPAT, IFIUDB, USPATFULL
           (*File contains numerically searchable property data)
```

```
Page 9
              1
       CM
       CRN 1493-13-6
       CMF CHF3 03 S
      - so<sub>3</sub>H
              2
       CM
       CRN
             62-53-3
       CMF C6 H7 N
          NH<sub>2</sub>
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
                    11 REFERENCES IN FILE CA (1907 TO DATE)
                    11 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
       ANSWER 789 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN 425-75-2 REGISTRY
L4
RN
       Entered STN: 16 Nov 1984
ED
       Methanesulfonic acid, trifluoro-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX
CN
       NAME)
OTHER NAMES:
       Ethyl triflate
CN
       Ethyl trifluoromethanesulfonate
CN
       Ethyl trifluoromethylsulfonate
CN
       Trifluoromethanesulfonic acid ethyl ester
CN
MF
       C3 H5 F3 O3 S
CI
       STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, TOXCENTER, USPATZ, USPATFULL (*File contains numerically searchable property data)

Other Sources: EINECS**, NDSL**, TSCA**

(**Enter CHEMITST File for up-to-data regulatory information)
       COM
LC
             (**Enter CHEMLIST File for up-to-date regulatory information)
          -CF3
Eto-
       Ö
```

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

```
197 REFERENCES IN FILE CA (1907 TO DATE)
               197 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
     ANSWER 790 OF 791 REGISTRY COPYRIGHT 2006 ACS on STN
L4
     358-23-6 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Methanesulfonic acid, trifluoro-, anhydride (6CI, 7CI, 8CI, 9CI) (CA
CN
OTHER NAMES:
     Perfluoromethanesulfonic anhydride
CN
     Tirflic anhydride
CN
     Triflate anhydride
CN
     Triflic acid anhydride
CN
     Triflic anhydride
CN
     Trifluoromethanesulfonic acid anhydride
CN
     Trifluoromethanesulfonic anhydride
CN
     Trifluoromethy]su]fonic acid anhydride.
CN
     Trifluoromethylsulfonic anhydride
CN
      93916-16-6
DR
MF
     C2 F6 O5 S2
CI
                    BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
LC
      STN Files:
        CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, GMELIN*, IFICDB, IFIPAT, IFIUDB, IPA, MSDS-OHS, PIRA, PROMT, PS, SYNTHLINE, TOXCENTER, USPATZ, USPATFULL (*File contains numerically searchable property data)
                         EINECS**, NDSL**, TSCA**
      Other Sources:
           (**Enter CHEMLIST File for up-to-date regulatory information)
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
              2021 REFERENCES IN FILE CA (1907 TO DATE)
              10 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 2026 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                 4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
      ANSWER 791 OF 791 REGISTRY COPYRIGHT 2006 ACS. on STN. ...
L4
      333-27-7 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
     Methanesulfonic acid, trifluoro-, methyl ester (6CI, 7CI, 8CI, 9CI) (CA
CN
      INDEX NAME)
OTHER NAMES:
      Methyl triflate
CN
      Methýl trifluoromethanesulfonate
CN
      NSC 270679
CN
      Trifluoromethanesulfonic acid methyl ester
CN
      C2 H3 F3 O3 S
MF
      COM
CI
        N Files: AGRICOLA, BEILSTEIN*, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CSCHEM, GMELIN*, MEDLINE, PIRA, PROMT,
      STN Files:
LC
        SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL
```

(\*File contains numerically searchable property data)
Other Sources: EINECS\*\*, NDSL\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

909 REFERENCES IN FILE CA (1907 TO DATE)
17 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
911 REFERENCES IN FILE CAPLUS (1907 TO DATE)
4 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d his

L1

L2

(FILE 'HOME' ENTERED AT 04:28:36 ON 11 DEC 2006)

FILE 'REGISTRY' ENTERED AT 04:39:37 ON 11 DEC 2006 STRUCTURE UPLOADED 2 S L1

L3 1206 SEARCH L1 FULL T91 S TRIFLATE

=> d 13 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200

L3 ANSWER 100 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN

RN 765886-51-9 REGISTRY

ED Entered STN: 20 Oct 2004

CN Zincate(1-), bis(2(3H)-benzothiazolethionato-xS2)(butanoato-xO)(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

MF C21 H24 N3 O2 S4 Zn

CI CCS, COM

SR CA

L3 ANSWER 200 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
RN 282549-07-9 REGISTRY
ED Entered STN: 02 Aug 2000
CN Cobalt(2+), tetraaqua(methanamine)(methanol)-, (OC-6-32)- (9CI) (CA INDEX NAME)

MF C2 H17 CO N O5

```
CCS
CI
SR
     CA
LC
     STN Files:
                   CA, CAPLUS
      он-ме
           OH<sub>2</sub>
H20.
          OH2
H20
      NH2-Me
                1 REFERENCES IN FILE CA (1907 TO DATE)
                1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
     ANSWER 300 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
L3
     149641-87-2 REGISTRY
Entered STN: 27 Aug 1993
Nickel(1+), (1-propanamine)- (9CI) (CA INDEX NAME)
RN
ED
CN
OTHER NAMES:
      (Propylamine) nickel (1+)
CN
     C3 H9 N Ni
MF
     CCS
CI
SR
     CA
                    CA, CAPLUS
     STN Files:
LC
H3C-CH2-CH2-NH2-Ni+
                1 REFERENCES IN FILE CA (1907 TO DATE)
                1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
     ANSWER 400 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN
L3
     132517-77-2 REGISTRY
RN
     Entered STN: 08 Mar 1991
ED
     Copper(2+), tetrakis(1-butanamine)-, diperchlorate (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
     1-Butanamine, copper complex C16 H44 Cu N4 . 2 Cl O4
CN
MF
SR
     STN Files:
                  CA, CAPLUS
LC
           1
     CM
          30904-66-6
     CRN
     CMF C16 H44 Cu N4
     CCI CCS
            NH2-Bu-n
             2+
                 -NH2-Bu-n
n-Bu-NH2-Cu-
            NH2-Bu-n
```

Page 12

```
Page 13
             2
      CM
      CRN 14797-73-0
      CMF C1 04
                    1 REFERENCES IN FILE CA (1907 TO DATE)
                    1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
      ANSWER 500 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN
L3
      110303-66-7 REGISTRY
Entered STN: 19 Sep 1987
RN
ED
      Copper(2+), triaqua(2-methyl-1-propanamine)-, (SP-4-2)- (9CI) (CA INDEX
CN
      NAME)
OTHER CA INDEX NAMES:
      1-Propanamine, 2-methyl-, copper complex C4 H17 Cu N O3
MF
CI
      CCS, COM
SR
      CA
       OH<sub>2</sub>
            - NH2— Bu-i
       OH<sub>2</sub>
      ANSWER 600 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN
L3
      91172-12-2 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
      Cobalt(2+), triaqua(1-propanamine)-, (T-4)-, (OC-6-22)-pentakis(cyano-C)nitrosylferrate(2-) (1:1), trihydrate (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
      1-Propanamine, cobalt complex
Ferrate(2-), pentakis(cyano-C)nitrosyl-, (OC-6-22)-, (T-4)-triaqua(1-
propanamine)cobalt(2+) (1:1), trihydrate (9CI)
C5 Fe N6 O . C3 H15 CO N O3 . 3 H2 O
STN Files: CA, CAPLUS
CN
CN
LC
      CM
             1
             91172-11-1
      CRN
             C5 Fe N6 O . C3 H15 CO N O3
       CMF
             CM
                    2
```

CRN 91172-10-0

CCS

CMF

CCI

C3 H15 CO N O3

L3 ANSWER 700 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN RN 68245-50-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Mercury, (1-butanamine)bis(cyano-C)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, mercury complex
MF C6 H11 Hg N3
CI CCS
LC STN Files: CA, CAPLUS

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
ANSWER 800 OF 1206 REGISTRY COPYRIGHT 2006 ACS on STN
L3
     56873-03-1 REGISTRY
RN
     Entered STN: 16 Nov 1984
     Mercury, diiodobis(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     2-Propanamine, mercury complex
OTHER NAMES:
     Mercuric iodide compound with isopropylamine (1:2)
     C6 H18 Hg I2 N2
MF
CI
     CCS
     STN Files: CA, CAPLUS
LC
```

```
NH2-Pr-i
               2 REFERENCES IN FILE CA (1907 TO DATE)
               2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
    ANSWER 900 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN
L3
     40231-90-1 REGISTRY
RN
    Entered STN: 16 Nov 1984
ED
    Zinc, dibromobis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
    1-Propanamine, 2-methyl-, zinc complex
CN
     C8 H22 Br2 N2 Zn
MF
     CCS
CI
     STN Files:
                 CA, CAPLUS
LC
          Br-
           2+
i-Bu-NH2-Zn-
               – NH2 — Bu-i
          Br-
               3 REFERENCES IN FILE CA (1907 TO DATE)
               3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
     ANSWER 1000 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN
L3
     30904-66-6 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Copper(2+), tetrakis(1-butanamine)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     1-Butanamine, copper complex
CN
     Copper(2+), tetrakis(butylamine)-, ion (8CI)
CN
OTHER NAMES:
     Tetrakis(butylamine)copper(2+)
CN
     Tetrakis(butylamine)copper(II)
CN
     C16 H44 Cu N4
MF
     CCS, COM
CI
     STN Files: CA, CAPLUS, GMELIN*
LC
         (*File contains numerically searchable property data)
           NH2-Bu-n
           2+
               – NH2 — Bu-n
           NH2-Bu-n
               3 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
               3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
     ANSWER 1100 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN
L3
```

RN

18901-59-2 REGISTRY

#### Page 16

ED Entered STN: 16 Nov 1984
CN Cuprate(2-), tetrachlorobis(methylamine)-, dihydrogen (8CI) (CA INDEX NAME)
MF C2 H10 Cl4 Cu N2 . 2 H
CI CCS
LC STN Files: CA, CAPLUS
CRN (795219-69-1)

●2 H+

LC

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 1200 OF 1206 REGISTRY COPYRIGHT 2006 ACS ON STN RN 13987-19-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(methylamine)bis(phthalimidato)- (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Copper, bis(phthalimidato)bis(methylamine)- (7CI)
MF C18 H18 Cu N4 O4
CI CCS

CA, CAOLD, CAPLUS

STN Files:

5 REFERENCES IN FILE CA (1907 TO DATE) 5 REFERENCES IN FILE CAPLUS (1907 TO DATE) 2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
Page 17
```

```
Uploading C:\Program Files\Stnexp\Queries\10749450a.str
        STRUCTURE UPLOADED
L5
=> d 15
L5 HAS NO ANSWERS
                STR
L5
G2
 CF3-OSO3H
G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu
G2 Ag,Cd,Co,Cu,Fe,Hg,Ni,Zn
Structure attributes must be viewed using STN Express query preparation.
=> s 15
SAMPLE SEARCH INITIATED 04:47:33 FILE 'REGISTRY'
                                        0 TO ITERATE
SAMPLE SCREEN SEARCH COMPLETED -
                                                                  0 ANSWERS
100.0% PROCESSED
                        0 ITERATIONS
SEARCH TIME: 00.00.01
                        ONLINE
                                 **COMPLETE**
FULL FILE PROJECTIONS:
                                 **COMPLETE**
                        BATCH
                                  0 TO
PROJECTED ITERATIONS:
PROJECTED ANSWERS:
                                  0 TO
              0 SEA SSS SAM L5
L6
Uploading C:\Program Files\Stnexp\Queries\10749450b.str
L7
        STRUCTURE UPLOADED
=> d 17
```

**L7** 

L7 HAS NO ANSWERS

STR

N<del>H2----</del>G1

G2

G3 S,P

G3 G1 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu G2 Ag,Cd,Co,Cu,Fe,Hg,Ni,Zn

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

=> s 17SAMPLE SEARCH INITIATED 04:49:18 FILE 'REGISTRY' 11364 TO ITERATE SAMPLE SCREEN SEARCH COMPLETED -

2000 ITERATIONS 17.6% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

**SEARCH TIME: 00.00.01** 

ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\* FULL FILE PROJECTIONS:

220892 TO 233668 PROJECTED ITERATIONS: 0 TO PROJECTED ANSWERS:

L8 0 SEA SSS SAM L7

=> search 17 ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:. ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET: Full FULL SEARCH INITIATED 04:49:31 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 228829 TO ITERATE

121 ANSWERS 100.0% PROCESSED 228829 ITERATIONS SEARCH TIME: 00.00.01

121 SEA SSS FUL L7 L9

=> file caplus SINCE FILE TOTAL COST IN U.S. DOLLARS **ENTRY SESSION** 394.62 390.84 FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 04:49:41 ON 11 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 11 Dec 2006 VOL 145 ISS 25 FILE LAST UPDATED: 10 Dec 2006 (20061210/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s 1946 L9 L10

=> d 110 fbib ab hitstr 1-46

ANSWER 1 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN

2004:344669 CAPLUS AN

141:81204 DN

Reversible and selective amine interactions of  $[Cd(\mu 2-N,0-p-m)]$ TI NH2C6H4SO3)2(H2O)2]n

ΑU

Zhou, Jin-Sen; Cai, Jiwen; Wang, Li; Ng, Seik-Weng School of Chemistry & Chemical Engineering, Sun Yat-Sen University,

Guangzhou, 510275, Peop. Rep. China Dalton Transactions (2004), (9), 1493-1497 CODEN: DTARAF; ISSN: 1477-9226 SO

Royal Society of Chemistry

PB Journal DT

LA English

CASREACT 141:81204 os

 $[Cd(\mu 2-N,0-p-NH2C6H4SO3)2(H2O)2]n$  (1) is a layered coordination compound AB The solid-vapor reactions between crystalline 1 and volatile amines were studied and the corresponding amine adducts were characterized by elemental anal., TGA, PXRD and IR. Among them, the C2H5NH2 and PrNH2 adducts, [Cd(C2H5NH2)4(H2O)2](H2NC6H4SO3)2 (3) and [Cd(PrNH2)4(O-p-H2NC6H4SO3)2] PrNH2 (4), grew into single crystals in situ from the solid-vapor reaction processes and their crystal structures were characterized. In both cases, 4 mol equivalent of amine mols. coordinate to Cd(II) via replacing the N,O-p-NH2C6H4SO3 ligands or coordinated H2O mols. The single-phase product suggests that the solid-vapor reaction between the metal sulfonate and volatile alkylamines could be used as a green process to synthesize monoamine-coordinated Cd(II) complexes without any solvent and routine separation Finally, the substitution reaction is reversible at room conditions and selective for primary alkylamines. IT

713079-80-2P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation via reversible solid-vapor coordinative substitution of layered cadmium(II) aminobenzenesulfonate aqua complex solid with volatile alkylamine, and crystal structure and TGA of)

### Page 20

RN CN

713079-80-2 CAPLUS Cadmium, bis(4-aminobenzenesulfonato- $\kappa$ 0)tetrakis(1-propanamine)-, (oC-6-12)-, compd. with 1-propanamine (1:1) (9CI) (CA INDEX NAME)

CM

713079-79-9 CRN

CMF C24 H48 Cd N6 O6 S2

CCI CCS

PAGE 1-A

PAGE 2-A

2 CM

CRN 107-10-8 CMF C3 H9 N

H3C-CH2-CH2-NH2

Page 20

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 36 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10

2003:613865 CAPLUS AN

140:357466 DN

Theoretical studies on C-heteroatom bond formation via reductive TI elimination from group 10 M(PH3)2(CH3)(X) species (X = CH3, NH2, OH, SH) and the determination of metal-X bond strengths using density functional theory

ΑU

MacGregor, Stuart A.; Neave, Greg W.; Smith, Christopher Department of Chemistry, School of Engineering and Physical Sciences, CS Heriot-Watt University, Edinburgh, EH14 4AS, UK Faraday Discussions (2003), 124, 111-127

SO CODEN: FDISE6; ISSN: 1359-6640

Royal Society of Chemistry PB

Journal DT LA Enalish

AB

D. functional calcns. were used to investigate C-C, C-N and C-O bond forming reactions via reductive elimination from Group 10 cis-[M(PH3)2(Me)(X)] species (X = Me, NH2, OH). Both direct reaction from the four-coordinate species and a three-coordinate mechanism involving initial PH3 loss was considered. For the four-coordinate pathway the ease of reductive elimination to give M(PH3)2 and Me-X follows the trend M=Pd < Pt < Ni. The reaction of the cis-M(PH3)2(Me)(NH2) species is promoted by the formation of methylamine adducts. Non-planar transition states are located and the C-heteroatom bond forming processes are characterized by migration of Me onto the cis-heteroatom ligand. For a given ligand, X, activation energies follow the trend M = Ni < Pd < Pt. Formation of the three-coordinate M(PH3)(Me)(X) species is promoted by a labilization of the cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OH. For the three-coordinate pathway the energy change for reductive elimination to give M(PH3) and Me-X again follows the trend M = Pd < Pt < Ni and in all cases the initial product is an M(PH3)(XMe) adduct. The three-coordinate transition states again involve migration of the Me ligand onto the cis-X ligand and for X = NH2 or OH activation energies follow the trend Ni > Pd < Pt. For a given metal activation energies in both the four- and three-coordinate pathways increase along the series Me both the Tour- and three-coordinate pathways increase along the series Me < NH2 < OH. These trends in activation energy can be rationalized in terms of the strength of M-Me/M-X bonding as long as the extent of geometrical distortion required to obtain the transition state geometry is taken into account. Further calcns. on cis-Pd(PH3)2(Me)(SH) suggest that the more common exptl. observation of C(sp3)-S compared to C(sp3)-O reductive elimination arises from the greater kinetic accessibility of the former process rather than an intrinsic thermodn. preference for C-S bond formation. By comparison, the calcns. indicate that C(sp3)-N reductive elimination should be feasible from Ni and Pd systems. DF calcns. are shown to reproduce the relative homolytic bond strengths determined exptl shown to reproduce the relative homolytic bond strengths determined exptl. for Pt-X bonds. In the cis-M(PH3)2(Me)(X) systems the M-Me homolytic bond strength increases down the group while for M-NH2 and M-OH bonds the trend is M = Ni ≈ Pd < Pt. M-NH2 and M-OH bonds are considerably stronger than M-Me bonds and the presence of a heteroatom ligand serves to weaken M-CH3 bonds even further.

682767-97-1, (Methanamine)bis(phosphine)nickel
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM
(Formation, nonpreparative); RACT (Reactant or reagent)
 (optimized geometry, potential energy, dissociation; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me

amido-, alkoxy- and mercapto-complexes) 682767-97-1 CAPLUS RN CN

Nickel, (methanamine)bis(phosphine)- (9CI) (CA INDEX NAME)

IT

```
PH<sub>3</sub>
H3P-Ni-NH2-CH3
      682768-13-4, (Methanamine)(phosphine)nickel
IT
      RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
      nonpreparative)
          (optimized geometry, potential energy; DFI geometry and energy profile
          of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
          mercapto-complexes)
      682768-13-4 CAPLUS
RN
      Nickel, (methanamine)(phosphine)- (9CI) (CA INDEX NAME)
CN
H3C-NH2-Ni 0 PH3
                 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 74
                 ALL CITATIONS AVAILABLE IN THE RE FORMAT
      ANSWER 3 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
L10
      2003:509917 CAPLUS
AN
DN
      139:77881
      Metal thioether complexes as organic metal precursors for use in forming
TI
      metal-containing patterned films
Jung, Won Cheol; Chang, Seok; Hwang, Soon Taik; Byun, Young Hun
IN
      Samsung Electronics Co., Ltd., S. Korea
PA
SO
      Eur. Pat. Appl., 8 pp.
      CODEN: EPXXDW
DT
      Patent
      English
LA
FAN. CNT 1
                               KIND
                                        DATE
                                                       APPLICATION NO.
                                                                                    DATE
      PATENT NO.
                                                                                    20021111
                                                       EP 2002-257784
                                Α2
                                        20030702
PΙ
      EP 1323721
      EP 1323721
                                        20031008
                                Α3
               AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
                                                       KR 2001-87510
                                                                                A 20011228
                                                                                    20011228
                                                       KR 2001-87510
                                        20030704
      KR 2003057133
                                                                                    20021029
                                                       us 2002-282031
      us 2003124457
                                        20030703
                                A1
                                        20051115
      us 6965045
                                 В2
                                                                                A 20011228
                                                       KR 2001-87510 -- -
                                                       JP 2002-373621
                                                                                    20021225
                                        20031010
      JP 2003286579
                                A2
                                                       KR 2001-87510
                                                                                A 20011228
      MARPAT 139:77881
os
      Disclosed are organic metal precursors comprising one or more thioether
AB
      ligands bonded to one or more metal atoms (metal = Ag, Au, Co, Cu, Pd, Ni, Pt, Zn, Cd), wherein the organic ligand is rapidly dissociated from the metal atom upon exposure to light and degraded leaving a metal or a metal oxide.
      Thus, reaction of AgNO2 and Et2S in heated MeCN afforded
      [(Et2s)Ag+](NO2-). Reaction of the latter with PrNH2 in MeCN afforded [(PrNH2)Ag]2SEt2. Using the organic metal precursors of the present
      invention, e.g., [(PrNH2)Ag]2SEt2, an electroconductive, metal-containing patterned film can be easily deposited on a substrate at room temperature under
      atmospheric pressure without using photosensitive resins.
      550305-04-9P
IT
```

```
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
        (Reactant or reagent)
             (preparation as precursor for use in forming metal-containing patterned
             photodegrdn. without use of photosensitive resins)
        550305-04-9 CAPLUS silver(2+), bis(1-propanamine)[\mu-[1,1'-thiobis[ethane]]]di-, dinitrite
RN
CN
        (9CI) (CA INDEX NAME)
        CM
                                                     ... .. .. ...
                 550305-03-8
        CRN
               C10 H28 Ag2 N2 S
        CMF
        CCI CCS
     Ag + NH2-Pr-n
Et-S-Et
     Aa+NH2-Pr-n
                 2
        CM
        CRN 14797-65-0
        CMF
                N 02
0 = N - 0^{-}
        ANSWER 4 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN
L10
        2003:472276 CAPLUS
AN
        139:239001
DN
        Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
TI
        Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China Journal of Materials Chemistry (2003), 13(7), 1806-1811 CODEN: JMACEP; ISSN: 0959-9428 Royal Society of Chemistry
ΑU
CS
S0
PB
DT
         Journal
        English
[Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered
LA
AB
        metal sulfonate. It can selectively intercalate ammonia and amines quant.
        without dehydration and form stable adducts, via solid-vapor reaction at
        without dehydration and form stable adducts, via solid-vapor reaction at room temperature. The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid
        in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed. The intercalation process is
        reversible, selective and preferential, indicating that the title compound
        could be designed as an amine-sensitive material.
```

```
Page 24
```

595548-10-0P 595548-12-2P 595548-14-4P IT 595548-16-6P 595548-18-8P 595548-20-2P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex) CAPLUS 595548-10-0 RN Cadmium, bis(methanamine)[1,5-naphthalenedisulfonato(2-)- $\kappa$ 0]-, compd. with methanamine (1:1), dihydrate (9CI) (CA INDEX NAME) CN CM 595548-09-7 CRN C12 H16 Cd N2 O6 S2 CMF CCI NH2-Me 503-2 CM CRN 74-89-5 CMF C H5 N H<sub>3</sub>C-NH<sub>2</sub> 595548-12-2 CAPLUS RN Cadmium, bis(ethanamine)[1,5-naphthalenedisulfonato(2-)- $\kappa$ 0]-, compd. CN with ethanamine (1:2), dihydrate (9CI) (CA INDEX NAME) CM 1 CRN 595548-11-1 CMF C14 H20 Cd N2 O6 S2 CCI CCS - NH2— Et

\$03<sup>-</sup>

```
Page 25
```

2 CM 75-04-7 CRN C2 H7 N CMF H3C-CH2-NH2 595548-14-4 CAPLUS Cadmium, [1,5-naphthalenedisulfonato(2-)- $\kappa$ 0]bis(1-propanamine)-, compd. with 1-propanamine (1:2), dihydrate (9CI) (CA INDEX NAME) RN CN  $\mathsf{CM}$ 595548-13-3 CRN C16 H24 Cd N2 O6 S2 CCI CCS NH2-Pr-n \_ | 2+ - cd -NH2-Pr-n SO3-2 CM 107-10-8 CRN CMF C3 H9 N H3C-CH2-CH2-NH2 595548-16-6 CAPLUS Cadmium, [1,5-naphthalenedisulfonato(2-)- $\kappa$ 0]bis(2-propanamine)-, compd. with 2-propanamine (1:1), dihydrate (9CI) (CA INDEX NAME) RN CN 1 CM

Page 25

CRN

CCI CCS

595548-15-5

CMF C16 H24 Cd N2 O6 S2

CM - 2

CRN 75-31-0 CMF C3 H9 N

RN 595548-18-8 CAPLUS
CN Cadmium, bis(1-butanamine)[1,5-naphthalenedisulfonato(2-)-κ0]-,
compd. with 1-butanamine (1:1), dihydrate (9CI) (CA INDEX NAME)

CM 1

CRN 595548-17-7 CMF C18 H28 Cd N2 O6 S2 CCI CCS

CM 2

CRN 109-73-9 CMF C4 H11 N

H3C-CH2-CH2-CH2-NH2

RN 595548-20-2 CAPLUS
CN Cadmium, bis(2-methyl-1-propanamine)[1,5-naphthalenedisulfonato(2-)KO]-, compd. with 2-methyl-1-propanamine (1:1), dihydrate (9CI) (CA
INDEX NAME)

```
1
CM
     595548-19-9
CRN
     C18 H28 Cd N2 O6 S2
CMF
    CCS
     NH2-Bu-i
- o - Cd - 2+
          -NH2—Bu-i
```

CM 2 CRN 78-81-9 C4 H11 N CMF

S03-

CH3 H3C- CH- CH2- NH2

L10

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 35 ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN

2002:283881 CAPLUS AN 137:84151 DN Activation volumes for a series of spontaneous, acid-and base-catalysed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, TI NO3-, SO42-)

Benzo, Fabian; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz ΑU Catedra de Quimica Inorganica, Facultad de Quimica, Universidad de la Republica, Montevideo, 11800, Urug. Inorganic Reaction Mechanisms (Amsterdam, Netherlands) (2001), 3(1), 25-29 CS

SO

CODEN: IRMEFE; ISSN: 1028-6624 Gordon & Breach Science Publishers PB DT Journal

English LA The vols. of activation for the spontaneous, base-, and acid- catalyzed The vols. of activation for the spontaneous, base-, and acid- catalyzed path of the hydrolysis reaction of a series of trans-[Co(MeNH2)(NH3)4X](3-n)+ ions (X = Cl-, Br-, (ONO2)- (OSO3)2-) have been determined in order to establish analogies with the dissociative trends found in previous work with the spontaneous hydrolysis of neutral ligands from the same cores. While for the base catalyzed path a significant decrease in the activation volume is found on going from the {Co(NH3)5} to the trans-{Co(MeNH2)(NH3)4} inert skeleton (i.e. 9.8, 12.5, 4.0 and 9.1 cm3mol-1 for the chloro, bromo, nitrato and sulfato derivs.), no significant changes are observed for the same complexes in the spontaneous reaction. The trends are AB the same complexes in the spontaneous reaction. The trends are rationalized in terms of the important changes occurring in

IT

and the important increase in the degree of dissociativeness due to the presence of a trans-methylamino ligand. For the acid catalyzed path the differences are much more difficult to assess, specially taking into account the limited information available as well as the inherent errors involved in the rate constant determination 210574-34-8

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-, NO3-, SO42-))
210574-34-8 CAPLUS

RN 210574-34-8 CAPLUS CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-k0]-, (OC-6-23)-(9CI) (CA INDEX NAME)

## RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 2000:445849 CAPLUS AN 133:49533 DN Aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobal TI t(III) complex ion Benzo, Fabian; Capparelli, Alberto L.; Martire, Daniel O.; Sienra, Beatriz ΑU Catedra de Quimica Inorganica, Facultad de Quimica, Montevideo, C.C.1157, CS Inorganic Reaction Mechanisms (Amsterdam) (2000), 1(4), 319-324 SO CODEN: IRMEFE; ISSN: 1028-6624 Gordon & Breach Science Publishers PB Journal DT English LA The kinetics of aquation and base hydrolysis reactions of AB trans-[Co(NH3)4(NH2CH3)(OSO3)]+ have been studied. In acid solution the aquation rate, Raq, follows the equation Raq/[complex] = ks + kc[H+], at constant ionic strength  $\mu$  = 1.0 M. The activation parameters are  $\Delta Hs\# = 88.8 \text{ kJ mol-1, } \Delta Ss\# = -50.5 \text{ JK-1 mol-1, } \Delta Hc\# =$ 96.7 kJ mol-1 and  $\triangle Sc\# = -23$  JK-1 mol-1. The rate consts. at 25°C are ks = 4.15 + 10-6 s-1 and kc = 4.52 M-1 s-1. The rate of base hydrolysis, ROH, follows the equation ROH/[complex] = kOH [OH-]. The activation parameters are  $\triangle HOH\# = 74.9 \text{ kJmol-1}$  and  $\triangle SOH\# = 2JK-1 \text{ mol-1}$  and the rate constant is kOH = 0.58 M-1 s-1 at 25°C and  $\mu$  = 0.15 M. The stereochem. of the hydroxo product has been determined (cis-[Co(NH3)4(NH2CH3)-(OH)]2+ = 9%). The results are discussed in the light of the reaction mechanisms proposed so far.

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT

(Reactant); PROC (Process); RACT (Reactant or reagent)

IT

210574-34-8

```
(aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatoc
            obalt(III) complex ion)
       210574-34-8 CAPLUS
RN
       Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-\kappa0]-, (OC-6-23)-
CN
        (9CI) (CA INDEX NAME)
         NH2-Me
             NH3
        Co 3+
               NH<sub>3</sub>
H<sub>3</sub>N
           _ so<sub>3</sub>-
                     THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 34
                     ALL CITATIONS AVAILABLE IN THE RE FORMAT
       ANSWER 7 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN
L10
       2000:398528 CAPLUS
AN
       133:79995
DN
       Inductive effect of methyl groups on acidopentaaminecobalt(III) complexes
TI
       Benzo, Fabian; Beyer, Lothar; Bozoglian, Fernando; Hallmeier, Karl-Heinz;
ΑU
       Sienra, Beatriz
       Universidad de la Republica, Catedra de Quimica Inorganica, Montevideo,
CS
       Polyhedron (2000), 19(8), 971-974
CODEN: PLYHDE; ISSN: 0277-5387
SO.
       Elsevier Science Ltd.
PB
        Journal
DT
LA
       English
       Electron spectroscopy for chemical anal. (ESCA) was performed for
AB
        [Co(NH3)5cl](Clo4)2, trans-[Co(NH3)4(NH2CH3)Cl]-(Clo4) 2
       [CO(NH3)5CI](CIO4)2, trans-[CO(NH3)4(NH2CH3)CI]-(CIO4) 2, [CO(NH2CH3)5CI](CIO4)2 and trans-[CO(NH3)4(NH2CH3)(OSO3)](CI O4) complexes. Comparison of the results for the complexes [CO(NH3)5CI](CIO4)2 and trans-[CO(NH3)4(NH2CH3)CI](CIO4)2 shows clearly the electronic influence (+I effect) of the methylamine group on the cobalt and through this on the chlorine atom in trans position. Comparison of [CO(NH2CH3)5CI](CIO4)2 with trans-[CO(NH3)4(NH2CH3)CI](CIO4)2 shows that methylation of the four cis-NH3 ligands does not produce a proportional decrease in the binding energy of the cobalt atom. While the electron d. of the chloro ligand is not
       the cobalt atom, while the electron d. of the chloro ligand is not affected. For the complex trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) the +I
        effect is almost completely compensated by the presence of the sulfato
        group in trans position. Acid dissociation consts. are also reported for [Co(NH3)5(OH2)]3+ and trans-[Co(NH3)4(NH2CH3)(OH2)]3+ ions. The
        implications of these results for the mechanism of the acid and base
        hydrolysis reactions of acidopentaaminecobalt(III) complexes are discussed. The preparation of the trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4)
        complex through the trans-[Co(NH3)4(NH2CH3)(SO3)]+ precursor is also
        described.
        279674-00-9
IT
        RL: PRP (Properties)
             (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
        279674-00-9 CAPLUS
RN
       Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-\kappa0]-, (OC-6-23)-,
CN
        perchlorate (9CI) (CA INDEX NAME)
```

1 CM

210574-34-8 CRN

CMF C H17 Co N5 O4 S

CCI CCS .

CM

CRN 14797-73-0

CMF C1 04

134066-32-3 IT

RL: RCT (Reactant); RACT (Reactant or reagent) (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)

134066-32-3 CAPLUS RN

Cobalt(1+), tetraammine(methanamine)[sulfito(2-)- $\kappa$ 0]-, (OC-6-23)-(9CI) (CA INDEX NAME) CN

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 32 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN 2000:22952 CAPLUS

```
DN
           Ab Initio calculations of [CoY6-nXn]2+ complexes Rulisek, Lubomir; Havlas, Zdenek
TI
ΑU
           Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic, Prague, 166 10, Czech Rep. Journal of Chemical Physics (2000), 112(1), 149-157 CODEN: JCPSA6; ISSN: 0021-9606 American Institute of Physics
CS
SO.
PB
DT
            Journal
            English
LA
           The CASSCF and multi-reference second order perturbation theory (CASPT2)
          The CASSCF and multi-reference second order perturbation theory (CASPT2) calcns. of [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes (X = CH3OH, CH3SH, CH3NH2) are reported. The potential energy surfaces of 10 lowest quartet states of [Co(H2O)5X]2+ complexes near the equilibrium geometry are calculated and splitting of triple-degenerate 4Tlg(F), 4T2g(F), and 4Tlg(P) electronic states of [Co(H2O)6]2+ complex induced by the substitution of one or two water ligands is characterized and quantified. The energy differences between originally degenerate states are almost invariant to the changes of metal-ligand distances, and despite their proximity, the crossing does not occur. The coeffs. of the leading configuration of multi-reference wave functions of [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes are shown to approach unity and the usage of single-reference methods is justified. As
AB
            approach unity and the usage of single-reference methods is justified. consequence, interaction energies of the studied functional groups with
           Co2+ are computed also at the HF, DFT and MP2 levels. They are compared to CASSCF calcns. and to the equivalent calcns. done for Zn2+ and Ni2+ ions.
           The computational methodol. for the accurate calcus. of various cobalt (II) ionic complexes is described and the implications for the theor. investigation of interactions of chemical and biol. important functional
            groups with Co2+ are discussed.
282547-96-0 284476-55-7
IT
            RL: PRP (Properties)
                    (ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+,
                    [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH,
                    CH3NH2))
            282547-96-0
                                          CAPLUS
RN
            Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-32)- (9CI) (CA
CN
            INDEX NAME)
              SH-Me
                     _OH2
              Ċo 2+
                       OH<sub>2</sub>
H20'
              NH2-Me
            284476-55-7 CAPLUS
RN
            Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-23)- (9CI) (CA
CN
            INDEX NAME)
```

# RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 9 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN
L10
          1999:759418
                                  CAPLUS
AN
          132:142592
DN
          Variable temperature and pressure study of the aquation reactions of
TI
          cobalt(III) and chromium(III) penta- and tetra-amines
         Benzo, Fabian; Bernhardt, Paul V.; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz
ΑU
          Facultad de Quimica, Catedra de Quimica Inorganica, Universidad de la
CS
          Republica, Montevideo, 11800, Urug.
Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry
SO
          (1999), (22), 3973-3979
CODEN: JCDTBI; ISSN: 0300-9246
          Royal Society of Chemistry
PB
          Journal
DT
          English
LA
          Preparation of a series of specific penta- and tetra-amine derivs. of CoIII and CrIII with a neutral leaving ligand has been carried out in order to
AB
          accomplish a fine tuning of the associativeness/dissociativeness of their
          substitution reactions. Spontaneous aquation reactions of the neutral
         ligands have been studied at variable temperature and pressure. Although ra consts. and thermal activation parameters show an important degree of scatter, the values determined for the activation vols. of the substitution process illustrate the mechanistic fine tuning that may be achieved for these reactions. In all cases, in the absence of important steric constraints in the mol., electronic inductive effects seem to be the most important factor accounting for the dissociative shifts observed both for pentaamine i.e. \Delta V.dbldag. = +4.0 or +14.0 cm3 mol-1 and +5.2 or +16.5 cm3 mol-1 for the aquation of cis- or trans-[Co(MeNH2)(NH3)4(DMF)]3+ and cis- or trans-[CoL15(DMF)]3+ resp., where L15 represents a pentaamine macrocyclic ligand, tetraamine systems i.e. \Delta V.dbldag. = +4.1 or +8.4 cm3 mol-1 and -10.8 or -7.4 cm3 mol-1 for the aquation of cis-[Co(NH3)4Cl(DMAC)]2+ (DMAC = dimethylacetamide) or
          ligands have been studied at variable temperature and pressure. Although rate
          cis-[Co(NH3)4Cl(DMAC)]2+ (DMAC = dimethylacetamide) or
         cis-[Co(en)2Cl(DMAC)]2+ and cis-[Cr(NH3)4Cl(DMF)]2+ or cis-[Cr(en)2Cl(DMF)]2+. From the results, clear evidence is obtained which indicates that, only when the situation is borderline Ia/Id, or the steric demands are increased dramatically, dissociative shifts are observed; in all other cases electronic inductive effects seem to be dominant for
          such a tuning of the substitution process.
          138521-43-4
IT
          RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
                (variable temperature and pressure study of aquation reactions of
cobalt(III)
                 and chromium(III) penta- and tetra-amines)
          138521-43-4 CAPLUS
RN
```

Cobalt(3+), tetraammine(methanamine)[(sulfinyl-k0)bis[methane]]-.

CN

(OC-6-23)- (9CI) (CA INDEX NAME)

## RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1999:702066 CAPLUS AN 132:36842 DN Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Mati Flexsys America LP, Akron, OH, USA CS Rubber Chemistry and Technology (1999), 72(2), 318-333 SO. CODEN: RCTEA4; ISSN: 0035-9475 American Chemical Society, Rubber Division PΒ Journal DT English LA vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic AB

sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.

15214-57-0 252564-24-2 252564-26-4

TT 15214-57-0 252564-24-2 252564-26-4 252564-27-5 252564-28-6 252564-30-0 252564-31-1 252564-34-4 252564-35-5 252564-36-6 252564-37-7 252564-38-8 252564-83-3

RL: MOA (Modifier or additive use); USES (Uses)... (insights into sulfur vulcanization from quant. structure-property relationships studies)

RN 15214-57-0 CAPLUS
CN Zinc, bis(2(3H)-benzothiazolethionato-kS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

### Page 34

RN 252564-24-2 CAPLUS
CN Zinc, bis(2(3H)-benzothiazolethionato-kS2)bis(2-propanamine)-,
(T-4)- (9CI) (CA INDEX NAME)

$$S \xrightarrow{N^{-}} S \xrightarrow{2+} Zn - NH_2 - Pr - i$$

$$NH_2 - Pr - i$$

RN 252564-26-4 CAPLUS
CN Zincate(1-), (butanoato-κο)(2-methyl-2-propanamine)bis(4(1H)-pyrimidinethionato-κ54)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

$$S-Z_{n}$$
 $S-Z_{n}$ 
 $S-Z_{n}$ 
 $S-Z_{n}$ 

● H+

RN 252564-27-5 CAPLUS Zinc, bis(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-KS2)-, (T-4)- (9CI) (CA INDEX NAME)

RN 252564-28-6 CAPLUS
CN Zincate(1-), (butanoato-ĸO)(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-κS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

● H+

RN 252564-30-0 CAPLUS
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-kS2)(butanoato-kO)(ethanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

● H+

RN 252564-31-1 CAPLUS
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-kS2)(butanoato-kO)(2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

Page 36

● H<sup>+</sup>

RN 252564-34-4 CAPLUS CN Zincate(1-), (butanoato-ĸO)(2-methyl-2-propanamine)bis(4-nitro-2(1H)-pyridinethionato-ĸS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

H+

RN 252564-35-5 CAPLUS
CN Zincate(1-), (butanoato-κ0)(2-methyl-2-propanamine)bis(2(1H)-pyrazinethionato-κ52)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

● H+

RN 252564-36-6 CAPLUS
CN Zincate(1-), (butanoato-κ0)(2-methyl-2-propanamine)bis(2(1H)-pyridinethionato-κ52)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

● н-1

RN 252564-37-7 CAPLUS
CN Zincate(1-), (butanoato-κο)(2-methyl-2-propanamine)bis(2(1H)-pyrimidinethionato-κs2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

● H<sup>+</sup>

RN 252564-38-8 CAPLUS
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κ0)(2-methyl-2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)

● H+

RN 252564-83-3 CAPLUS
CN Zinc, bis(4,6-dimethyl-2(1H)-pyrimidinethionato-kS2)bis(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 11 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN
L10
         1999:645540 CAPLUS
ΑN
DN
        An organometallic route to zinc phosphonates and their intercalates Gerbier, Philippe; Guerin, Christian; Henner, Bernard; Unal, Jean-Remi U.M.R. 5637 -Universite Montpellier II, Montpellier, 34095, Fr. Journal of Materials Chemistry (1999), 9(10), 2559-2565
         132:8432
TI
ΑU
CS
50
        CODEN: JMACEP; ISSN: 0959-9428
Royal Society of Chemistry
PB
         Journal
DT
         English
LA
         An organometallic nonaq. route to zinc phosphonates and to their
AB
         intercalates was studied. Various phosphonic acids react with
        dimethylzinc in THF media to afford the corresponding layered zinc phosphonates Zn(O3PR1) (R1 = Me, Ph, 2- and 3-thienyl, thiophen-3-ylmethyl) with evolution of methane. The presence of a primary n-alkylamine in the reaction mixture allows the 1-pot formation of
         2-dimensional-layered intercalated phases Zn(03PR1) RNH2 [R2 = Bu, Penn (n-pentyl)] whereas a more bulky amine such as cyclohexylamine (HexcNH2) give 1-dimensional polymeric chains Zn(03PPh)·2HexcNH2. 162050-26-2P 184824-62-2P
IT
         RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
               (preparation from organometallic nonaq. route, interlayer spacing and 31P CP
              MAS NMR spectrum of intercalate)
         162050-26-2 CAPLUS
RN
```

CN Zinc, (1-butanamine)[phenylphosphonato(2-)-ĸ0]- (9CI) (CA INDEX NAME)

RN 184824-62-2 CAPLUS CN Zinc, (1-butanamine)[methylphosphonato(2-)-κ0]- (9CI) (CA INDEX NAME)

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 12 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1998:433445 CAPLUS AN 129:141178 DN Competition study for the base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ TI Benzo, Fabian; Mendoza, Carolina; Queirolo, Marcelo; Sienra, Beatriz Quimica Inorganica, Facultad de Quimica, Montevideo, Urug. Polyhedron (1998), 17(13-14), 2295-2299 CODEN: PLYHDE; ISSN: 0277-5387 ΑU CS SO Elsevier Science Ltd. PB Journal DT English LA Nitrite ion competition has been measured for the base hydrolysis reaction AΒ of trans-Co(N-H3)4(NH2CH3)Xn+ ions (X = Cl-, Br-, NO3- and SO42-) in 1.0 M NANO2 at 25°C. Both 0- and N- bonded Co(NH3)4(NH2CH3)NO22+ are formed. Subsequently the Co(NH3)4(NH2CH3)ONO2+ isomer rearranges in OH-to give the thermodynamically more stable Co(NH3)4(NH2CH3)NO22+ ion. The total NO2- captured shows a slight dependence on the overall charge of the complex and on the nature of X (R = 2.2, 2.1, 3.6 and 1.2±0.5% for X = Cl-, Br-, NO3- and SO42-, resp.). These results differ from those observed with complexes of the type Co(NH3)5Xn+ and Co(NH2CH3)5Xn+ where X includes a variety of anions. 210574-34-8 IT RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (competition study for base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+ complexes)

RN 210574-34-8 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-κ0]-, (OC-6-23)(9CI) (CA INDEX NAME)

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1997:809063 CAPLUS AN 128:146849 DN Infrared and Raman spectra of Na2Cu(SO4)2.2H2O and TI  $(CH3NH3)2M(II)(SO4)2 \cdot 6H2O \text{ with } M(II) = Cu, Zn, and Ni$ Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B. Department of Physics, St. Gregorios College, Kottarakara, 691531, India Journal of Solid State Chemistry (1997), 133(2), 407-415 CODEN: JSSCBI; ISSN: 0022-4596 ΑU CS **SO** PB Academic Press Journal DT

English LA FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2.6H2O with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order. AB the order, (CH3NH3) Cu(s04)2.6H20 > (CH3NH3)2Ni (s04)2.6H20 > (CH3NH3)2Zn(S04)2·6H20 > Na2Cu(S04)2·2H20. The appearance of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and S042- groups. The appearance of multiple bands in the between NH3 and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mole. in strong hydrogen bonds involving water mols. in (CH3NH3)2Cu(SO4)2·6H2O and (CH3NH3)2 Zn(SO4)2·6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2·6H2O.
202406-44-8 202406-47-1 202406-49-3 IT RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process) (IR and Raman spectra, internal vibrational mode assignments, and hydrogen bonding) 202406-44-8 CAPLUS RN Cuprate(2-), bis(methanamine)bis[sulfato(2-)- $\kappa$ 0]-, dihydrogen, hexahydrate (9CI) (CA INDEX NAME)

CN

●2 H+

●6 H<sub>2</sub>0

202406-47-1 CAPLUS RN Zincate(2-), bis(methanamine)bis[sulfato(2-)- $\kappa$ 0]-, dihydrogen, hexahydrate, (T-4)- (9CI) (CA INDEX NAME)

●2 H+

●6 H<sub>2</sub>O

RN 202406-49-3 CAPLUS
CN Nickelate(2-), bis(methanamine)bis[sulfato(2-)-κ0]-, dihydrogen, hexahydrate (9CI) (CA INDEX NAME)

●2 H+

●6 H2O

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 14 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 ΑN 1996:704546 CAPLUS DN 126:41873 Structure of Zn(03PC2H4CO2H) 0.5C6H5NH2 and XANES-EXAFS study of TI the intercalation of amines into Zn(O3PR) H2O zinc alkylphosphonates Drumel, Stephanie; Janvier, Pascal; Bujoli-Doeuff, Martine; Bujoli, Bruno ΑU IMN, UMR CNRS 110, Faculte des Sciences et des Techniques, Nantes, 44072, CS Journal of Materials Chemistry (1996), 6(11), 1843-1847 CODEN: JMACEP; ISSN: 0959-9428 SO Royal Society of Chemistry PB Journal DT LA English

AB From XANES-EXAFS expts., neither the dehydration nor the subsequent n-alkylamine intercalation in Zn(O3PCH3)·H2O appears to be topotactic. On the contrary, the whole process consists of breaking Zn-O bonds present in the hydrated material, so that no bridging oxygen remains in the inorg. sheet. This hypothesis is supported by the structural determination

IT

of an aniline intercalate: Zn(O3PC2H4CO2H)·0.5C6H5NH2 [orthorhombic, space group Pbcn, a 29.880(6), b 8.526(2), c 14.720(3) A, Z = 16, R = 0.043 and Rw = 0.047; 2063 observed reflections, I > 2σ(I)]. For steric reasons, only half of the zinc atoms are coordinated to aniline; the 2nd half of the metal atoms that are not bound to the amine retain the environment present in the initial anhydrous phase. 184824-62-2 RL: PRP (Properties)

(XANES-EXAFS spectra of)

184824-62-2 CAPLUS RN

Zinc, (1-butanamine)[methylphosphonato(2-)-x0]- (9CI) (CA INDEX CN

$$n-Bu-NH_2-Zn\frac{2+}{-}0-P-Me$$

ANSWER 15 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10

1996:652255 CAPLUS ΑN

125:286037 DN

Quantum-chemical studies on the mechanism of the novel reaction of TI oxidative amination of P4 in the copper(II) coordination sphere

ΑU

Dorfman, Ya. A.; Abdreimova, R. R. Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy of Sciences of Kazakhstan, Almaty, Kazakhstan

Russian Journal of Coordination Chemistry (Translation of SO Koordinatsionnaya Khimiya) (1996), 22(10), 716-729 CODEN: RJCCEY: ISSN: 1070-3284

PB MAIK Nauka/Interperiodica

DT Journal

AΒ

English LA

A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NRZ)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II) → Cu(O) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intraand interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions. 182930-87-6 182930-88-7 182930-94-5

IT

182930-97-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (quantum-chemical studies on mechanism of oxidative amination of P4 in constant of the constant

copper(II) coordination sphere)
RN 182930-87-6 CAPLUS
CN Cuprate(2-), tetrachloro(methanamine)(phosphine)-, (OC-6-32)- (9CI) (CA INDEX NAME)

RN 182930-94-5 CAPLUS CN Copper(1+), triaquachloro(methanamine)(phosphine)-, (OC-6-43)- (9CI) (CA INDEX NAME)

RN 182930-97-8 CAPLUS CN Copper(2+), triaquabis(methanamine)(phosphine)-, (OC-6-22)- (9CI) (CA INDEX NAME)

```
ANSWER 16 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
L10
        1996:130370 CAPLUS
AN
        125:24833
DN
        Interaction of copper powder with nonaqueous solutions of methylammonium
TI
        Babich, O. A.; Kokozei, V. N.; Pavlenko, V. A.
Kiev. Gos. Univ., Kiev, Ukraine
Zhurnal Neorganicheskoi Khimii (1996), 41(1), 79-82
ΑU
CS
SO
        CODEN: ZNOKAQ: ISSN: 0044-457X
PB
        MAIK Nauka
        Journal
DT
LA
        Russian
        The interaction of Cu powder with MeCN, MeOH, DMSO, and DMF solns. of
AB
       methylammonium bromide, iodide, or thiocyanate was studied. Products of the interaction were isolated and identified. The crystalline structure of [Cu(CH3NH2)4]I2 was detd (monoclinic, P21/n, a = 7.088(1), b = 8.872(1), C = 10.590(1) Å, \beta = 95.29(1)°, V = 663.04 Å3, Z = 2, \rhoC = 2.212 g/cm3, \mu(CuK\alpha) = 390.3 cm-1, F(000) = 414, T = 20^{\circ}, 1043 reflections with I > 3\sigma(I), R = 0.061, Rw = 0.090).
        57286-68-7P
IT
        RL: SPN (Synthetic preparation); PREP (Preparation)
             (preparation from Cu and methylammonium salts in nonaq. solns.)
        57286-68-7 CAPLUS
RN
        Copper, bis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
CN
            Me-NH2
                 2+
               - cu--- v--- c--- s
```

```
ANSWER 17 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN
L10
                          CAPLUS
        1996:10558
AN
        124:128031
DN
        Outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
TI
       complexes. A temperature- and pressure-dependence kinetic study on the effects of the different {N5} groups
Martinez, Manuel; Pitarque, Mari-Angel
Facultat Quimica, Universitat Barcelona, Barcelona, E-08028, Spain
ΑU
        Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry
SO
        (1995), (24), 4107-11
        CODEN: JCDTBI; ISSN: 0300-9246
        Royal Society of Chemistry
PB
```

Me-NH2

Journal DT English

English
Outer-sphere redox reactions between [Co{N5}(HnPO4)]n+[{N5} = (NH3)5,
(NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane (L)] and
[Fe(CN)6]4- have been studied as a function of pH, {N5}, temperature and
pressure. The effect of the size of the {N5} skeleton, has been
investigated for the n = 0, 1, 2 systems in order to establish possible
correlations between the size and charge of the cobalt(III) complex and
the ion-pair formation constant, the electron-transfer rate constant, and the
thermal and baric activation parameters. The values obtained indicate LA AB thermal and baric activation parameters. The values obtained indicate that the ion-pair formation consts. are the same, within exptl. error, for all the systems studied. The electron-transfer rate constant for a given degree (n = 1) of protonation of the  $[Co\{N5\}(HnPO4)]n+ complex increases$ on increasing the size of the monodentate amines, while an important decrease is observed when they are substituted by the N5 macrocycle (L) [2.6 + 10-3 s-1, {N5} = (NH3)5, 59 + 10-3 s-1, {N5} = (NH2Me)5, 0.73 + 10-3 s-1, {N5} = L; resp. at 35°C]. The activation enthalpies do not show any significant change, neither with decreasing enthalpies do not show any significant change, neither with decreasing charge on the cobalt complex nor with the size of the amine. The values of  $\Delta S$ .thermod. and  $\Delta V$ .thermod. vary considerably with the degree of protonation of the phosphate ligands and the size of the CoIII cavity of the complexes. The opposite trends observed for the values of  $\Delta S$ .thermod. [8 J K-1 mol-1 for {N5} = (NH2Me)5 (n = 1); -61 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 32 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 17 cm3 mol-1 for {N5} = (NH3)5 (n = 0)] are related to the existence of an important increase in hydrogen bond formation in the cobalt(III) complex important increase in hydrogen bond formation in the cobalt(III) complex on going to the transition state.

173178-22-8 173178-23-9 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] IT complexes and temperature- and pressure-dependence kinetic effects of different {N5})

173178-22-8 CAPLUS Cobalt, pentakis (methanamine) [phosphato(3-)-0]-, conjugate monoacid, (OC-6-22)-(9CI) (CA INDEX NAME)

RN

CN

● H<sup>+</sup>

173178-23-9 CAPLUS Cobalt, pentakis(methanamine)[phosphato(3-)-0]-, (OC-6-22)- (9CI) (CA RN CN INDEX NAME)

ANSWER 18 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1995:899304 CAPLUS ΑN 124:67877 DN Coordinative intercalation of alkylamines into layered zinc TI phenylphosphonate. Crystal structures from x-ray powder diffraction data Poojary, Damodara M.; Clearfield, Abraham Department of Chemistry, Texas AM University, College Station, TX, 77843, ΑU CS USA Journal of the American Chemical Society (1995), 117(45), 11278-84 **SO** CODEN: JACSAT: ISSN: 0002-7863 American Chemical Society PB DT Journal English LA Zn phenylphosphonate monohydrate takes up 1 mol of amine when contacted with liquid primary alkylamines. The mechanism of intercalation involves AB replacement of the coordinated H2O mol. by the amine mols. Although the composition of the intercalate Zn(O3PPh)(RNH2) is consistent with the anal. and spectroscopic data, there exist discrepancies in the observed interlayer d spacings of the intercalate with respect to that in the host compound The d spacing for the propylamine intercalate is in fact smaller than that in Zn phenylphosphonate itself. To understand this feature specifically and to explain the mechanism of amine intercalation in metal phosphonates in general the authors determined the structures of the intercalates. The general, the authors determined the structures of the intercalates. The structures of Zn(O3PPh)(RNH2), R = -C3H9 (1), -C4H11 (2), -C5H13 (3), were solved ab initio from x-ray powder diffraction data and refined by solved ab initio from x-ray powder diffraction data and refined by Rietveld methods. All the compds. are isostructural, and they crystallize in the monoclinic space group P21/c with a 13.978(3), b 8.791(2), c 9.691(2) Å, and  $\beta$  102.08(1)° for 1, a 14.698(4), b 8.957(3), c 9.712(3) Å, and  $\beta$  102.465(3)° for 2, and a 16.267(3), b 8.935(2), c 9.695(2) Å, and  $\beta$  102.32(1)° for 3. The structures of these intercalates are new and are different from that of the host compound although all of them are layered. In the intercalate the Zn atoms are tetrahedrally coordinated as opposed to octahedral coordination in the host compound 162050-25-1P 162050-26-2P 162050-25-1P 162050-26-2P IT RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

Zinc, [phenylphosphonato(2-)-0](1-propanamine)- (9CI) (CA INDEX NAME)

162050-25-1 CAPLUS

(preparation and crystal structure of)

RN

CN

162050-26-2 CAPLUS RN Zinc, (1-butanamine)[phenylphosphonato(2-)-κ0]- (9CI) (CA INDEX CN ANSWER 19 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1995:676435 CAPLUS ΑN DN 123:102111 Zinc sulfadiazines: novel topical antimicrobial agents for burns TI Lee, A. R.; Huang, W. H. Sch. Pharmacy, National Defense Med. Cent., Taipei, Taiwan ΑU CS Journal of Pharmacy and Pharmacology (1995), 47(6), 503-9 CODEN: JPPMAB; ISSN: 0022-3573
Royal Pharmaceutical Society of Great Britain 50 PB DT Journal English LA Two new zinc sulfadiazine (Zn(SD)2)-amine complexes, zinc AB sulfadiazine-methylamine (Zn(SD)2(CH3NH2)2) and zinc sulfadiazineethylenediamine (Zn(SD)2(C2H8N2)3.H2O), were prepared and compared with silver sulfadiazine (AgSD). The compds. were readily obtained by reaction of zinc nitrate hexahydrate with sulfadiazine or its methylamine and ethylenediamine salts. Structure was established by X-ray crystallog. and UV-visible, IR and NMR spectroscopy. The products were effective, in-vitro, against Gram-pos. and Gram-neg. bacteria as well as fungus. However, their activity is partially reversed by p-aminobenzoic acid. Further investigations in burned mice revealed that these compds. displayed a potential value in the prevention and treatment of wound healing, and diminution of mortality and weight loss. The toxicity of Zn(SD)2 derivs. was much lower than that of AgSD. The better aqueous solubility and skin permeability may explain the reason for their superiority over AgSD in the efficacy for topical therapy. Zn(SD)2(CH3NH2)2 was consistently more potent and was chosen for further development in clin. The similarity in complexation between Sn(SD)2(CH3NH2)2 and AgSD may be significant to distinguish that from any other Zn(SD)2 derivative in bioactivity. 126830-36-2P IT RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)\_\_\_ (zinc sulfadiazines and novel topical antimicrobial agents for burns)

Zinc, bis(4-amino-N-2-pyrimidinylbenzenesulfonamidato)bis(methanamine)-,

RN

CN

126830-36-2 CAPLUS

(T-4)-(9CI) (CA INDEX NAME)

ANSWER 20 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1995:419353 CAPLUS ΑN 122:229146 DN Intercalation of alkylamines into dehydrated and hydrated zinc TI phenylphosphonates Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham Department of Chemistry, Texas A and M Univ., College Station, TX, 77843, ΑU CS USA Journal of Materials Chemistry (1995), 5(2), 315-18 **SO** CODEN: JMACEP; ISSN: 0959-9428 Royal Society of Chemistry PB Journal DT English LA Primary amines, CnH2n+1NH2 (n = 3-8), were intercalated into layered AB anhydrous Zn phenylphosphonate Zn(O3PPh) and its monohydrate Zn(O3PPh).H2O when the host compds. were brought into contact with liquid amines. In both cases, 1 mol of amine was intercalated forming layered compds. Zn(O3PPh).(RNH2) as characterized by powder x-ray diffraction, TG and IR spectroscopy. The amines coordinate to the Zn atoms at the site vacated by the H2O mol. A plot of the interlayer distances of the intercalates vs. the number of C atoms in the alkyl chain of the amine gives a straight line with a slope of 1.24 Å, which indicates that the alkyl chains are most likely packed as an interdigitated monolayer with a tilt angle of 78° with respect to the mean plane of the layer. A comparison of the intercalation reactions of Zn, Co and Cu Me- and phenyl-phosphonates

is included in the discussion section. 162050-25-1P 162050-26-2P IT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

162050-25-1 CAPLUS RN

Zinc, [phenylphosphonato(2-)-0](1-propanamine)- (9CI) (CA INDEX NAME) CN

162050-26-2 CAPLUS RN Zinc, (1-butanamine)[phenylphosphonato(2-)-κ0]- (9CI) (CA INDEX CN NAME)

ANSWER 21 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1993:234154 CAPLUS ΑN 118:234154 DN Intercalation of alkylamines into layered copper phosphonates Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
Chemistry of Materials (1993), 5(4), 495-9 TI ΑU CS 50 CODEN: CMATEX; ISSN: 0897-4756 DT Journal English Dehydration of layered copper phosphonates Cu(O3PR):H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. LA AB of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(03PCH3) and Cu(03PCH5). The copper methylphosphonate takes up 1 mol of amine forming Cu(03PCH3) (RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates 141848-52-4P 147578-74-3P 147578-79-8P IT 147578-80-1P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and interlayer distances of)

RN 141848-52-4 CAPLUS CN Copper, (1-butanamine)[methylphosphonato(2-)-0]- (9CI) (CA INDEX NAME)

RN 147578-74-3 CAPLUS CN Copper, [methylphosphonato(2-)-0](1-propanamine)- (9CI) (CA INDEX NAME)

$$n-Pr-NH_2-Cu-0-P-Me$$

RN 147578-79-8 CAPLUS CN Copper, [phenylphosphonato(2-)-0]bis(1-propanamine)- (9CI) (CA INDEX NAME)

147578-80-1 CAPLUS RN Copper, bis(1-butanamine)[phenylphosphonato-0]- (9CI) (CA INDEX NAME) CN

ANSWER 22 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10

1992:419105 CAPLUS AN

117:19105 DN

Synthesis, crystal structures, and coordination intercalation behavior of two copper phosphonates TI

ΑU

Zhang, Yiping; Clearfield, Abraham Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA CS

Inorganic Chemistry (1992), 31(13), 2821-6 CODEN: INOCAJ; ISSN: 0020-1669 S0

Journal DT

English LA Cu(03PMe).H20 and Cu(03PPh).H20 were synthesized and their structures AB determined Cu(03PMe).H20 is monoclinic: space group P21/c, a 8.495(4), b 7.580(4), c 7.289(4) Å,  $\beta$  90.08 (4)°, Z = 4, R = 0.030, RW = 0.041. The structure is layered as formed by unusual 5-coordinate distorted tetragonal pyramidal Cu atoms. One O of each phosphonate bonds to 2 Cu atoms forming a chain, while the other 2 phosphonate 0 atoms bond to 2 Cu atoms in an adjacent chain. The base of the pyramid consists of 3 phosphonate 0 atoms and the coordinated H20 mol. All H bonds are of the intralayer type, so only van der Waals forces exist between adjacent layers. Amines are coordinatively intercalated with layer expansion. Cu(03PPh).H20 is orthorhombic: space group Pbca, a 7.5547(4), b 7.4478(6), c 27.928(1) Å, Z=8, R=0.037 and Rw=0.043. The coordination about the Cu atoms and the layer structure are identical to those of the O3PMe compound The Ph rings in the interlamellar space are oriented at a 98° angle to each other in adjacent rows. These structures are compared to those of other layered divalent phosphonates and Cu phosphites. IT

141848-52-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and interlayer spacing of intercalation compound)

141848-52-4 CAPLUS RN Copper, (1-butanamine) [methylphosphonato(2-)-0]- (9CI) (CA INDEX NAME) CN

$$n-Bu-NH_2-Cu-2+0-P-Me$$

```
ANSWER 23 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     1992:50338 CAPLUS
AN
     116:50338
DN
     Synthesis and characterization of trans-[Co(NH3)4(NH2CH3)L]3+[L=
TI
      (CH3)2SO or (CH3)2NCHO] complexes
     Sienra, Beatriz; Massaferro, Adriana
ΑU
     Fac. Quim., Montevideo, Urug. Polyhedron (1991), 10(17), 2075-8 CODEN: PLYHDE; ISSN: 0277-5387
CS
SO
DT
      Journal
     Enalish
LA
     trans-[Co(NH3)4(NH2Me)Me2SO]X3 (X = ClO4, Br) and trans-
AB
      [CO(NH3)4(NH2Me)Me2NCHO](Cl04)3 are prepared by Ag+-induced solvolysis of
     trans-[Co(NH3)4(NH2Me)X]^{2+} (X = Cl or Br) complexes in DMSO or DMF. The complexes were characterized by electronic, IR and 1H NMR. DMSO and DMF
     are bonded through the oxygen atom. The trans-complexes obtained are not
      contaminated with the cis-isomers.
      138521-44-5P 138521-45-6P
IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
      138521-44-5 CAPLUS
RN
      Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-0]-, (OC-6-23)-,
CN
      triperchlorate (9CI) (CA INDEX NAME)
      CM
           1
           138521-43-4
      CRN
           C3 H23 Co N5 O S
      CMF
      CCI
           CCS
              NH3
      H<sub>3</sub>N
Me-NH2
              `мнз
       H3N
                  Me
            2
      CM
           14797-73-0
      CRN
            cl 04
      CMF
      138521-45-6 CAPLUS
RN
      Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-0]-, tribromide,
CN
```

(OC-6-23)- (9CI) (CA INDEX NAME)

●3 Br-

```
ANSWER 24 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN.
L10
     1991:258445 CAPLUS
AN
     114:258445
DN
     Synthesis, characterization and some reactions of trans-
TI
     tetraamminebromo(methanamine)cobalt(2+) and trans-
     tetraammine(methanamine(nitratocobalt(2+) complexes
     Sienra, B.; Massaferro, A.; Piriz Mac-Coll, C. R.
Univ. Republica, Montevideo, Urug.
ΑU
CS
     Zeitschrift fuer Anorganische und Allgemeine Chemie (1990), 590, 222-8
SO
     CODEN: ZAACAB; ISSN: 0044-2313
     Journal
DT
     English
LA
     The preparation of trans-[Co(NH3)4(CH3NH2)Br]2+ (I) and trans-
ΑB
     [Co(NH3)4(CH3NH2)(NO3)]2+ is described. The UV-visible spectra of the
     complexes indicate a decrease of the ligand field compared to the parent
     pentaammines. IR spectra match with the pattern of the corresponding pentaammines. The catalyzed (by Hg2+) aquation of I occurred with
     retention of the stereochem. configuration. The base hydrolysis (studied
     at 25°) products show trans to cis rearrangement for both
     complexes. 1H NMR spectroscopy is used for identification of the
     stereochem. configuration of the compds.
     134066-33-4P, trans-Tetraammine(methylamine)sulfitocobalt(1+)
IT
     nitrate
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (preparation and decomposition of, in presence of nitric acid)
     134066-33-4 CAPLUS
RN
     Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-0]-, (OC-6-23)-, nitrate
CN
     (9CI) (CA INDEX NAME)
     CM
           1
     CRN 134066-32-3
     CMF C H17 CO N5 O3 S
     CCI
         CCS
```

CM 2

CRN 14797-55-8 CMF N 03

RN 134066-26-5 CAPLUS
CN Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-0]-, bromide, (OC-6-23)(9CI) (CA INDEX NAME)

● Br<sup>-</sup>

L10 ANSWER 25 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1990:209715 CAPLUS
DN 112:209715
TI A facile synthesis of zinc sulfadiazine derivatives
AU Lee, An Rong; Huang, Wen Hsin; Lai, Jin Shing; Chan, Shu Fei
CS Sch. Pharm., Natl. Def. Med. Cent., Taipei, Taiwan

Zhonghua Yaoxue Zazhi (1989), 41(4), 345-8 SO CODEN: CYHCEX; ISSN: 1016-1015

DT Journal

LA Enalish

Treatment of sulfadiazine with Zn(NO3)2 in the presence of NH4OH, MeNH2, AB or H2NCH2CH2NH2 gave the corresponding title complexes, whose mol. structures were determined

126830-36-2P IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mol. structure of)

126830-36-2 CAPLUS RN

zinc, bis(4-amino-N-2-pyrimidinylbenzenesulfonamidato)bis(methanamine)-, CN (T-4)-(9CI) (CA INDEX NAME)

ANSWER 26 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10

1987:584014 CAPLUS AN

107:184014 DN

Study of the bond strength in complex compounds by proton NMR TI

Galitskaya, S. M.; Pavlenko, L. I. ΑU

CS

Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6 SO CODEN: VLPIAZ; IŠSN: 0460-0436

DT Journal

Russian LA

Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN, NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases in the order CN > NCS # NCSe.  $\frac{10945-33-0}{38255-54-8}$   $\frac{110945-33-0}{10946-24-2}$ AB

IT

RL: PRP (Properties)
(bond energy in, NMR in study of)

38255-54-8 CAPLUS RN

Cadmium, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX CN NAME)

110945-33-0 CAPLUS RN Zinc, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME) CN

```
Page 55
```

RN 110946-24-2 CAPLUS CN Mercury, bis(1-butanamine-N)bis(thiocyanato-S)-, (T-4)- (9CI) (CA INDEX NAME)

```
ANSWER 27 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN 1986:507276 CAPLUS 105:107276
L10
AN
DN
       Pentakis (methanamine) (trifluoromethanesulfonato-0) complexes of
TI
       chromium(III), cobalt(III), and rhodium(III)
Lawrance, Geoffrey A.; Sargeson, Alan M.
ΑU
       Dep. Chem., Univ. Newcastle, 2308, Australia Inorganic Syntheses (1986), 24, 279-82 CODEN: INSYA3; ISSN: 0073-8077
CS
SO
DT
       Journal
       English
LA
       [M(NH2Me)5(0S02CF3)](S03CF3)2 (M = Co, Cr, Rh) were prepared from
AΒ
        [M(NH2Me)5Cl]Cl2 and CF3SO3H.
       90065-88-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from cobalt chloro methylamine complex and
IT
            trifluoromethanesulfonic acid)
       90065-88-6 CAPLUS
RN
       Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-0)-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX
CN
       NAME)
       CM
               1
       CRN 84254-64-8
       CMF C6 H25 C0 F3 N5 O3 S CCI CCS
```

2 CM CRN 37181-39-8 CMF C F3 03 S

L10

ANSWER 28 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN 1986:141030 CAPLUS AN DN 104:141030 Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) TI complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile Curtis, Neville J.; Lawrance, Geoffrey A.
Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia
Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669 ΑU CS S0 Journal DT Enalish LA Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile AB and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. As.thermod. and AV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis (methylamine) complexes. These results parallel earlier observations of \( \Delta S. \text{thermod. and} \) ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed. 100681-45-6P 100681-49-0P 100681-50-3P IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

Page 56

```
Page 57
```

CM 2

CRN 37181-39-8

CMF C F3 03 S

RN 100681-49-0 CAPLUS Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-0]-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)

CM 1

CRN 100681-48-9 CMF C7 H31 CO N5 O S CCI CCS

```
Page 58
          2
     CM
     CRN 37181-39-8
     CMF C F3 03 S
     S03-
     100681-50-3 CAPLUS Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-0]-, (OC-6-22)-,
RN
CN
     triperchlorate (9CI) (CA INDEX NAME)
          1
     CRN 100681-48-9
     CMF C7 H31 CO N5 O S
     CCI CCS
      Me-NH2 NH2-Me
      Me-NH2 NH2-Me
   Me
          2
     CM
     CRN 14797-73-0
     CMF C1 04
IT
     90065-88-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (substitution reactions of, with neutral ligands)
     90065-88-6 CAPLUS
RN
CN
```

90065-88-6 CAPLUS
Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-0)-,
(OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 84254-64-8
CMF C6 H25 CO F3 N5 O3 S

CCI CCS

CM 2

CRN 37181-39-8 CMF C F3 O3 S

ANSWER 29 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1986:121904 CAPLUS AN 104:121904 DN Formation and transformation of amminecarbonatocobalt(III) complexes TI Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R. Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth. Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40 CODEN: ZAACAB; ISSN: 0044-2313 ΑU CS 50 Journal DT English LA [COCO3(NH3)5]Clo4.H20, trans-[CoCO3(NH3)4(15NH3)]Clo4, and AB trans-[CoCO3(NH3)4(NH2Me)]Clo4 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. The products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific. 100788-52-1P 100838-96-8P 100838-97-9P IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, from carbonato complex in acidified DMSO) 100788-52-1 CAPLUS Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-0]-, (OC-6-44)- (9CI) (CA INDEX NAME) RN CN

100838-96-8 CAPLUS RN Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-0]-, CN (OC-6-43)- (9CI) (CA INDEX NAME)

100838-97-9 CAPLUS Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-0]-, (OC-6-34)- (9CI) (CA INDEX NAME) RN CN

ANSWER 30 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10

1986:96513 CAPLUS ÁN

104:96513 DN

Hydrolysis of coordinated trifluoromethanesulfonate from cobalt(III), TI

rhodium(III), iridium(III) and chromium(III) pentaamines
Curtis, Neville J.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan ΑU

Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia Inorganic Chemistry (1986), 25(4), 484-8
CODEN: INOCAJ; ISSN: 0020-1669 CS

SO

DT Journal

LA English Base hydrolysis and aquation of M(NH3)5(OSO2CF3)2+ (M = Co, Rh, Ir, Cr) and M(NH2CH3)5(OSO2CF3)2+ (M = Co, Rh, Cr) complexes at 25° and ionic strength 1.0 M are reported. The N-methylation of the ammine ligand AB causes a marked enhancement of the rate of base hydrolysis reactions with kMe/kH of 2100 (Co), 150 (Rh), and 800 (Cr). Only minor enhancements

occur for aquation with Co and Rh, while there is a minor rate diminution with Cr. Pos. activation entropies for base hydrolysis of M(NH3)5(OSO2CF3)2+ (M = Co, Ir) and competition expts. with azide ion in basic solution as well as the absence of the competing ion in the rate law allow a dissociative conjugate-base mechanism for all complexes. The variation in rate enhancement from ammine to methylamine compds. and the competition studies in base with azide ion chiefly reflect differences in steric interactions due to differing metal-ligand bond lengths rather than any mechanistic diversity. Variations in competition behavior for RhIII), Cr(III), and Co(III) appear to reflect relative lifetimes of the intermediate of reduced coordination number. The variations in aquation are much smaller and do not allow any certainty in mechanistic assertions. Marked accelerations of rates for both acid and base hydrolyses (.apprx.103-106-fold) occur consistently for all trifluoromethanesulfonato complexes compared with those of halo of analogs. 84254-64-8

RN 84254-64-8 CAPLUS CN Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-0)-, (OC-6-22)- (9CI) (CA INDEX NAME)

ANSWER 31 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1984:521855 CAPLUS AN 101:121855 DN synthetically versatile (trifluoromethanesulfonato)metal amine complexes TI Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan ΑU Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia CS Inorganic Chemistry (1984), 23(19), 2940-7 CODEN: INOCAJ; ISSN: 0020-1669 50 DT Journal English LA Facile preparation routes to complexes of the labile unidentate coordinated -OSO2CF3 ion are reported for M(NH3)5(OSO2CF3)n+ (M = Rh, Ir, Cr, Ru, n = 2, M = Pt, n = 3), M(NH2Me)5(OSO2CF3)2+ (M = Co, Rh, Cr), ΑB cis-M(en)2(OSO2CF3)2+ (M = Rh, Ir, Cr, and trans-M(en)2Cl(OSO2CF3)+ (M = Rh, Ir). The utility of these synthetically versatile intermediates in the preparation of a variety of complexes containing neutral ligands is illustrated. Rate consts. for the aquation of the triflato complexes in 0.1M CF3so3H at 25° span 3 orders of magnitude and for the pentaammine complexes show a reactivity order of Ru > Co .apprx. Cr .apprx. Rh » Ir > Pt. For the pentakis(methylamine) complexes, the aquation rate is greater for Co, slightly greater for Rh, and smaller for

Cr in comparison to the corresponding pentaammine complexes. The aquations of M(en)2X(OSO2CF3)+ proceed largely without isomerization (<5%), and the triflato complexes are prepared stereospecifically by this route. For the cis-M(en)2(OSO2CF3)2+ ions, consecutive 1st-order aquation processes are observed with rate consts. k1 .apprx. 2k2.

90065-88-6P IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and kinetics of aquation of)

90065-88-6 CAPLUS RN

Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-0)-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX CN NAME)

CM 1

CRN 84254-64-8

CMF C6 H25 Co F3 N5 O3 S

CCI CCS

2 CM

37181-39-8 CRN CMF C F3 03 S

ANSWER 32 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10

1983:100163 CAPLUS AN

DN 98:100163

(Trifluoromethanesulfonato-o)pentaammine complexes: versatile synthetic TI intermediates

Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan ΑU

Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia Inorganic Chemistry (1983), 22(5), 846-7 CS

SO

CODEN: INOCAJ; ISSN: 0020-1669

Journal DT

```
ANSWER 33 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     1980:153821 CAPLUS
AN
     92:153821
DN
     Complexing of copper(II) salts with pyridines and primary aliphatic amines
TI
     in dimethyl sulfoxide
     Dulova, V. I.; Brezhe, A. L.; Molchanova, N. R.; Artyukhova, E. P.
ΑU
     Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
Koordinatsionnaya Khimiya (1980), 6(2), 248-51
CS
SO
     CODEN: KOKHDC: ISSN: 0132-344X
     Journal
DT
     Russian
LA
     Instability consts. were determined spectrophotometrically and heats of
AB
     coordination were determined calorimetrically for 1:1 and 1:2 complexes by
     assuming equilibrium of the type Cu(DMSO)62+ + 2L .dblharw. Cu(DMSO)5L2+ +
     DMSO; Cu(DMSO)5L2+ + L .dblharw. Cu(DMSO)4L22+ + DMSO. The relative
     importance of bonding in these complexes is discussed.
     73358-71-1P 73358-73-3P
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation)
         (formation of, in DMSO)
     73358-71-1 CAPLUS
RN
                , bis(1-butanamine)tetrakis[sulfinylbis[methane]-0]- (9CI) (CA
     Copper(2+),
CN
     INDEX NAME)
```

RN 73358-73-3 CAPLUS Copper(2+), bis(2-methyl-2-propanamine)tetrakis[sulfinylbis[methane]-0]-(9CI) (CA INDEX NAME)

```
ANSWER 34 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN 1978:452589 CAPLUS
L10
AN
DN
      New tetrathiocyanatodiaminechromates with aliphatic monoamines
TI
      Ganescu, I.; Varhelyi, C.; Futo, F.; Brinzan, G.
ΑU
      Chem. Fak., Univ. Craiova, Craiova, Rom.
Zeitschrift fuer Anorganische und Allgemeine Chemie (1978), 439, 282-8
CS
S0
      CODEN: ZAACAB; ISSN: 0044-2313
      Journal
DT
      German
LA
      [\underline{Cr(NCS)4L2}] - (L = PrNH2, BuNH2) were prepared by a substitution_reaction of
AB
      K3[Cr(NCs)6] with L in the molten state. Twenty complex salts of the type
      R.H[Cr(NCS)4L2] (L = amine) and 20 Co-amine complexes with [Co(NCS)4L2]-were isolated. The complexes were characterized by IR and UV spectra.
      67008-64-4P 67008-65-5P
IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (preparation of)
      67008-64-4 CAPLUS Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-
RN
CN
      N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-
```

propanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 66915-22-8

CMF C10 H18 Co N6 S4

CCI CCS

CM 2

CRN 30649-39-9

CMF C18 H36 CO N4 O2

CCI CCS

PAGE 1-A

PAGE 2-A

RN 67008-65-5 CAPLUS

CN Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-butanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 66915-23-9

CMF C12 H22 Co N6 S4

CCI CCS

$$S = C = N$$
 $N = C = S$ 
 $N = C = S$ 

CM 2

CRN 30649-39-9

CMF C18 H36 CO N4 O2

CCI CCS

PAGE 1-A

PAGE 2-A

```
ANSWER 35 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
L10
        1977:83070 CAPLUS
ΑN
        86:83070
DN
       Heterogeneous reactions of solid nickel(II) complexes. X.
TI
        stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
       Jona, E.; Vojtas, B.; Sramko, T.
Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
Chemicke Zvesti (1976), 30(1), 107-13
ΑU
CS
S0
        CODEN: CHZVAN; ISSN: 0366-6352
        Journal
DT
       Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to
        English
LA
AB
        stereochem. changes in the coordination polyhedra. 61896-84-2P 61896-86-4P
IT
        RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (formation and thermal decomposition of)
        61896-84-2 CAPLUS
RN
        Nickel, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
CN
        NAME)
        CM
                1
        CRN 61896-83-1
        CMF C4 H10 N4 Ni S2
        CCI CCS
                NH2-Me
           2+
                NH2-Me
        61896-86-4 CAPLUS
RN
        Nickel, bis(ethanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
CN
        NAME)
        CM
                1
                61896-85-3
        CRN
        CMF
                C6 H14 N4 Ni S2
        CCI CCS
Et-NH2-
```

IT 61896-80-8P 61896-82-0P

```
Page 68
```

RL: PREP (Preparation) (formation, x-ray diffraction and thermal decomposition of) 61896-80-8 CAPLUS RN Nickel, tris(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX CN NAME) 1 CMCRN 61896-79-5 CMF C5 H15 N5 Ni S2 CCI CCS Me-NH2 NH2-Me 61896-82-0 CAPLUS RN Nickel, (methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX CN NAME) CM 1 CRN 61896-81-9 CMF C3 H5 N3 Ni S2 CCI CCS NH2-Me 61876-10-6 61914-81-6 IT RL: RCT (Reactant); RACT (Reactant or reagent) (thermal decomposition of) 61876-10-6 CAPLUS RN Nickel, tetrakis(ethanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA CN INDEX NAME)

Et-NH2 
$$N=C=S$$
NH2-Et
NH2-Et
NH2-Et

61914-81-6 CAPLUS RN Nickel, tetrakis(methanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA CN

INDEX NAME)

Me-NH2 NH2-Me

Me-NH2-Ni
$$\frac{2+}{N}$$
 N=C-S

Me-NH2 N=C-S

ANSWER 36 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1977:83011 CAPLUS AN 86:83011 DN Isomerism of nickel(II) complexes. VIII. Study of isomerism of TI isothiocyanatonickel(II) complexes with some alkylamines Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J.
Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352 ΑU CS S0 Journal DT English LA Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2Me)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the AB monomer isomerizes to the green pseudooctahedral polymer. Steric effects in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic spectra. 61876-10-6P 61896-84-2P 61896-86-4P IT 61914-81-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 61876-10-6 CAPLUS RN

Nickel, tetrakis(ethanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA

N = C = SEt-NH<sub>2</sub>

NH<sub>2</sub>-Et

Ni 2+

INDEX NAME)

Et-NH<sub>2</sub> NH<sub>2</sub>-Et

RN 61896-84-2 CAPLUS
CN Nickel, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 61896-83-1 CMF C4 H10 N4 Ni S2

CN

CCI CCS

61896-86-4 CAPLUS RN Nickel, bis(ethanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX CN NAME)

1 CM

61896-85-3 CRN C6 H14 N4 Ni S2 CMF CCI CCS

61914-81-6 CAPLUS RN Nickel, tetrakis(methanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA CN INDEX NAME)

Me- NH2 NH2-Me

Me- NH2-Ni
$$^2$$
+ N= C= S

Me- NH2 N= C= S

ANSWER 37 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10

1976:571027 CAPLUS AN

85:171027 DN

Copper(II) aminothiocyanates and aminoselenocyanates TI

ΑU

CS

Skopenko, V. V.; Savitskii, V. N. Kiev. Gos. Univ., Kiev, USSR Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg. SO Khim., Novosibirsk, USSR. CODEN: 34BFAN

DT Conference

LA Russian

Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Culater has a square bipyramidal configuration and the AB bipy, phen), the Cu atom has a square bipyramidal configuration and the

XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)z has a square bipyramidal environment.

60865-90-9P 60865-92-1P 60865-94-3P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

60865-90-9 CAPLUS

RN Copper, bis(1-propanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA CN INDEX NAME)

CM 1

60865-89-6 CRN C8 H18 Cu N4 S2 CMF CCS CCI

60865-92-1 CAPLUS RN Copper, bis(1-butanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX CN NAME)

1 CM

60865-91-0 CRN C10 H22 Cu N4 S2 CMF CCI CCS

60865-94-3 CAPLUS RN Copper, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX CN NAME)

1 CM

60865-93-2 CRN C4 H10 Cu N4 S2 CMF CCI CCS

ANSWER 38 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10

1976:425322 CAPLUS AN

85:25322 DN

The cobaltous amine reaction. II. Cobalt complexes of barbiturates, methimazole, methylthiouracil, naphazoline, phenytoin, sulfathiazole and TI theophylline

ΑU

Bult, Á. Lab. Pharm. Anal. Chem., State Univ. Groningen, Groningen, Neth. Pharmaceutisch Weekblad (1976), 111(17), 385-93 CS

S0 CODEN: PHWEAW; ISSN: 0031-6911

DT Journal

LA English

The complexes of the composition CoX2(amine)2(X = anion of barbital,The complexes of the composition COXZ(amine)Z(X = anion of barbital, hexobarbital, methylphenobarbital, pentobarbital, phenobarbital, theophylline, and sulfathiazole; amine = isobutylamine, isopropylamine or NH3) are pseudo tetrahedral (Co(II) complexes. Co(II) coordinates with the barbiturates via N-I, with theophylline via N-7 or N-9, with sulfathiazole via the tertiary N atom of the thiazole ring. With X = anion of phenytoin the octahedral complex Co(II)X2(amine)4 is formed. This pink complex dissolves CHCl3 to a violet tetrahedral complex. With a large excess of amine the tetrahedral is converted to an octahedral. AB large excess of amine the tetrahedral is converted to an octahedral. large excess of amine the tetranedral is converted to an octanedral. The donor atom in X is N-3. With X = naphazoline the (pseudo) tetrahedral Co(II) complexes CoX2(acetate)2 and [CoX4](ClO4)2 are prepared. The post charge of Co2+ is compensated by acetate (coordinated) and ClO4-(uncoordinated resp. The donor atom in X is the tertiary Atom. With use of the ir spectra of previously described Co(II) complexes of methimazole a contribution to the interpretation of the ir spectrum of this drug is given. With X = anion of methylthiouracil some Co(III) complexes with the average composition CoX2(amine)n (n = .apprx.3) are prepared. The lable data available data

are insufficient for assigning the structure. 59710-34-8P

IT

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and mol. structure of)

59710-34-8 CAPLUS RN

Cobalt, bis(4-amino-N-2-thiazolylbenzenesulfonamidato-NN)bis(2-methyl-1-CN propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

ANSWER 39 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN 1975:587668 CAPLUS AN 83:187668 DN Copper(II) aminothiocyanates and aminoselenocyanates TI Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V. ΑU Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8 CS SO CODEN: UKZHAU; ISSN: 0041-6045 DT Journal Russian Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2, RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes LA AB except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded. The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are N-bonded. 57286-68-7P 57286-70-1P 57286-71-2P IT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

Me- NH<sub>2</sub>

- | 2+ - | C- S

S-- C- N- Cu- N- C- S

| Me- NH<sub>2</sub>

57286-68-7 CAPLUS

RN 57286-70-1 CAPLUS CN Copper, bis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)

Copper, bis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)

RN

CN

57286-71-2 CAPLUS RN Copper, bis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME) CN

ANSWER 40 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10

1975:38050 CAPLUS 82:38050 ΑN

DN

Nickel aminothiocyanates and aminoselenocyanates TI

Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A. ΑU

Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32 CS SO

CODEN: UKZHAU; ISSN: 0041-6045

DT Journal

Amines in MeOH were added to MeOH solns. containing KSCN or KSeCN and Ni(NO3)2.6-H2O to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in Russian LA AB [NiL(NCX)]NCX. The magnetic moments of the complexes were determined

54438-97-0P 54438-99-2P 54439-01-9P IT RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

54438-97-0 CAPLUS RN

Nickel, tetrakis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME) CN

Me-NH2 NH2-Me

Me-NH2-Ni
$$\frac{2+}{N}$$
-C-S

Me-NH2 N-C-S

54438-99-2 CAPLUS RN Nickel, tetrakis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME) CN

$$\begin{array}{c|c}
 & -Pr-NH2 & NH2-Pr-n \\
 & NH2-Pr-n \\
 & NH2-Pr-n \\
 & NH2-Pr-n \\
 & -C=S
\end{array}$$

RN 54439-01-9 CAPLUS CN Nickel, tetrakis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)

ANSWER 41 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1974:530234 CAPLUS ΑN 81:130234 DN Chemistry of substituted sulfuric acids. VIII. Methanesulfonates of TI tin(II), tin(IV), and zinc(II)
Paul, Ram C.; Kapila, V. P.; Sharma, S. K. ΑU Dep. Chem., Panjab Univ., Chandigarh, India CS Indian Journal of Chemistry (1974), 12(6), 651-2 SO CODEN: IJOCAP; ISSN: 0019-5103 DT Journal LA English SnC12(MeSO3)2, Sn(MeSO3)2, and Zn(MeSO3)2 were prepared by reacting the resp. metal chlorides with MeSO3H. Their 1:2 adducts with pyridine and AB BUNH2 were prepared and their conductances studied in MeSO3H. The presence of phases Cs2M(MeSO3)4 (M = Sn or Zn) was indicated by f.p. detns. of the M(MeSO3)2-CsMeSO3 systems. 53396-13-7P IT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 53396-13-7 CAPLUS RN Zinc, bis(1-butanamine)bis(methanesulfonato-0)-, (T-4)- (9CI) (CA INDEX CN

NAME)

ANSWER 42 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1972:520272 CAPLUS ΑN 77:120272 DN Cadmium aminothiocyanates and aminoselenocyanates TI Skopenko, V. V.; Galitskaya, S. M. Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11 ΑU CS SO CODEN: UKZHAU; ISSN: 0041-6045 Journal DT Russian LA The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu, AΒ do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to the Cd atom via the N atom. 38255-49-1 38255-51-5 38255-54-8 IT 38441-98-4 RL: PRP (Properties) (ir spectrum of, structure in relation to) 38255-49-1 CAPLUS RN Cadmium, bis(methanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX CN

NAME)

RN 38255-51-5 CAPLUS CN Cadmium, bis(ethanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)

RN 38255-54-8 CAPLUS CN Cadmium, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)

RN 38441-98-4 CAPLUS
CN Cadmium, bis(1-propanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)

ANSWER 43 OF 46 CAPLUS COPYRIGHT 2006 ACS ON STN L10 1972:442560 CAPLUS AN DN 77:42560 Nitro methylamine complexes of cobalt(III) TI Ganiev, A. G.; Tukhtaev, Sh. Sh.; Ikramov, Kh. U. Inst. Yad. Fiz., Kiev, USSR ΑU CS Zhurnal Neorganicheskoi Khimii (1972), 17(5), 1384-7 50 CODEN: ZNOKAQ; ISSN: 0044-457X DT Journal Russian LA MeNH2 reacts with [Co(NO2)6]3- to give mixed complexes. K[Co(MeNH2)2(NO2)4], (CN3H5)H[Co(MeNH2)2(NO2)4], [Co(MeNH2)3(NO2)3], AB [Co(MeNH2)3(NO2)2(NCS)], [Co(MeNH2)2(NH3)(NO2)3], [Co(MeNH2)4(NO2)2][Co(NH3)2(NO2)4] were prepared The complexes of MeNH2 are less stable than the analogous NH3 complexes. 36741-31-8P IT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 36741-31-8 CAPLUS RN Cobalt, tris(methanamine)bis(nitrito-N)(thiocyanato-N)- (9CI) (CA INDEX CN

L10 ANSWER 44 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1971:544420 CAPLUS
DN 75:144420
TI Stepwise adduct formation of bis(0,0'-diethyldithiophosphato)nickel(II)
with primary and secondary amines

Ciullo, G.; Furlani, C.; Sestili, L.; Sgamellotti, A. ΑU Inst. Gen. Inorg. Chem., Univ. Perugia, Perugia, Italy Inorganica Chimica Acta (1971), 5(3), 489-92 CS SO CODEN: ICHAA3: ISSN: 0020-1693 DT Journal Enalish LA Bis(0,0'-diethyldithiophosphato)nickel(II) behaves in a qual. similar way AB with both primary and secondary amines in that 1:1 and 1:2 adducts are found. Data obtained for butylamine and diethylamine indicate that the difference in behavior towards primary and secondary amines is only quant., formation consts. being much smaller with the latter. Very high concn of primary amines leads also to the formation of complexes containing the chromophore (Nis2N4), presumably with monodentate dithiophosphate ligands. 34406-41-2 IT RL: PRP (Properties); FORM (Formation, nonpreparative) (formation consts. of) 34406-41-2 CAPLUS RN Nickel, tetrakis(butylamine)bis(dihydrogen phosphorodithioato)-, CN 0,0,0,0-tetraethyl ester (8CI) (CA INDEX NAME)

ANSWER 45 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10 1970:91917 CAPLUS AN 72:91917 DN Separation of aromatic hydrocarbons using metal-organic complexes TI Csikos, Rezso; Farkas, Peter ΑU CS Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10, SO 107-16 CODEN: MAFKAJ; ISSN: 0506-807X DT Journal Hungarian LA Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their AB selectivity, and stability were examined 27910-87-8 27910-88-9 28067-98-3 IT RL: USES (Uses) (in benzene derivative separation from heptane) 27910-87-8 CAPLUS RN

Nickel, tetrakis(ethylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME) CN

27910-88-9 CAPLUS RN Nickel, tetrakis(propylamine)bis(thiocyanato) - (8CI) (CA INDEX NAME) CN

28067-98-3 CAPLUS RN Nickel, tetrakis(isopropylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME) CN

ANSWER 46 OF 46 CAPLUS COPYRIGHT 2006 ACS on STN L10

1966:33012 CAPLUS AN

64:33012 DN

OREF 64:6075d

Vulcanization accelerator-activator complexes. I. Amine complexes of zinc and cadmium benzothiazole-2-thiolate

Milligan, Brian ΑU

Nat. Rubber Producers' Res. Assoc., Welwyn Garden City, UK CS J. Chem. Soc., Inorg., Phys., Theoret. (1966), (1), 34-5 SO

Journal DT

English LA Eleven amine complexes of Zn benzothiazole-2-thiolate were prepared from the AΒ NH3 complex. Dissociation of the pyridine complex provides a convenient route

=> => Uploading C:\Program Files\Stnexp\Queries\10749450c.str

L11 STRUCTURE UPLOADED

=> d 111 L11 HAS NO ANSWERS L11 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \* Structure attributes must be viewed using STN Express query preparation.

=> s l11
 REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 05:07:25 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 81 TO ITERATE

. 100.0% PROCESSED 81 ITERATIONS SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
1081 TO 2159

PROJECTED ITERATIONS: PROJECTED ANSWERS:

0 TO 0

L12 0 SEA SSS SAM L11

L13

0 L12

=> search 111 **REGISTRY INITIATED** 

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 05:07:34 FILE 'REGISTRY' **81 TO ITERATE** SAMPLE SCREEN SEARCH COMPLETED -

100.0% PROCESSED

**81 ITERATIONS** 

**O ANSWERS** 

**SEARCH TIME: 00.00.01** 

FULL FILE PROJECTIONS:

ONLINE \*\*COMPLETE\*\* \*\*COMPLETE\*\* BATCH

PROJECTED ITERATIONS:

2159 1081 TO

PROJECTED ANSWERS:

0 TO

L14

O SEA SSS SAM L11

0 L14 L15

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL

**SESSION ENTRY** 645.28

FULL ESTIMATED COST

0.46

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

**TOTAL** SINCE FILE **SESSION ENTRY** 

CA SUBSCRIBER PRICE

0.00 -34.50

FILE 'REGISTRY' ENTERED AT 05:07:39 ON 11 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

10 DEC 2006 HIGHEST RN 915124-84-4 STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4 DICTIONARY FILE UPDATES:

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

```
=> s 111
SAMPLE SEARCH INITIATED 05:07:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                          81 TO ITERATE
                                                                       O ANSWERS
100.0% PROCESSED
                         81 ITERATIONS
SEARCH TIME: 00.00.01
                          ONLINE **COMPLETE**
FULL FILE PROJECTIONS:
                                  **COMPLETE**
                          BATCH
                                              2159
                                 1081 TO
PROJECTED ITERATIONS:
                                                 0
                                    0 TO
PROJECTED ANSWERS:
               O SEA SSS SAM L11
ı 16
=> search 111
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 05:07:50 FILE 'REGISTRY'
                                      1257 TO ITERATE
FULL SCREEN SEARCH COMPLETED -
                                                                       0 ANSWERS
100.0% PROCESSED
                       1257 ITERATIONS
SEARCH TIME: 00.00.01
               0 SEA SSS FUL L11
L17
=> FIL STNGUIDE
                                                                       TOTAL
                                                      SINCE FILE
COST IN U.S. DOLLARS
                                                           ENTRY
                                                                     SESSION
                                                          167.82
                                                                      813.10
FULL ESTIMATED COST
                                                                       TOTAL
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                      SINCE FILE
                                                           ENTRY
                                                                     SESSION
                                                                       -34.50
                                                             0.00
CA SUBSCRIBER PRICE
FILE 'STNGUIDE' ENTERED AT 05:09:39 ON 11 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Dec 8, 2006 (20061208/UP).
=> d his
      (FILE 'HOME' ENTERED AT 04:28:36 ON 11 DEC 2006)
     FILE 'REGISTRY' ENTERED AT 04:39:37 ON 11 DEC 2006
                 STRUCTURE UPLOADED
L1
               2 S L1
L2
            1206 SEARCH L1 FULL
L3
             791 S TRIFLATE
L4
                  STRUCTURE UPLOADED
L5
               0 S L5
L6
                 STRUCTURE UPLOADED
L7
               0 S L7
L8
             121 SEARCH L7 FULL
L9
     FILE 'CAPLUS' ENTERED AT 04:49:41 ON 11 DEC 2006
              46 S L9
L10
                  STRUCTURE UPLOADED
L11
```

S L11

FILE 'REGISTRY' ENTERED AT 05:07:25 ON 11 DEC 2006 L12 0 S L11

FILE 'CAPLUS' ENTERED AT 05:07:26 ON 11 DEC 2006 L13 0 S L12 S L11

FILE 'REGISTRY' ENTERED AT 05:07:33 ON 11 DEC 2006 L14 0 S L11

FILE 'CAPLUS' ENTERED AT 05:07:34 ON 11 DEC 2006 L15 0 S L14

FILE 'STNGUIDE' ENTERED AT 05:09:39 ON 11 DEC 2006

=> d l10 all
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:n

=> file reg TOTAL SINCE FILE COST IN U.S. DOLLARS **ENTRY** SESSION 814.36 1.26 FULL ESTIMATED COST SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) **SESSION ENTRY** 0.00 -34.50 CA SUBSCRIBER PRICE

FILE 'REGISTRY' ENTERED AT 05:22:17 ON 11 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4 DICTIONARY FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

.=> d l9 1-121 all

```
L9 ANSWER 1 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN

RN 791764-59-5 REGISTRY

ED Entered STN: 03 Dec 2004

CN Nickelate(2-), bis(methanamine)bis[sulfato(2-)-k0]- (9CI) (CA INDEX NAME)

MF C2 H10 N2 Ni 08 S2

CI CCS, COM

SR CA
```

```
L9 ANSWER 2 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 788144-09-2 REGISTRY
ED Entered STN: 25 Nov 2004
CN Zincate(1-), (butanoato-κ0)(2-methyl-2-propanamine)bis(2(1H)-pyrimidinethionato-κ52)-, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 O2 S2 Zn
CI CCS, COM
SR CA
```

### Ring System Data

EA	ES	SZ	Ring System Formula RF	ן אַזט	Count
			+========   C4N2	46.195.24	2

```
L9 ANSWER 3 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 774525-06-3 REGISTRY
ED Entered STN: 04 Nov 2004
CN Zincate(1-), (butanoato-κ0)(2-methyl-2-propanamine)bis(4-nitro-2(1H)-pyridinethionato-κ52)-, (T-4)- (9CI) (CA INDEX NAME)
MF C18 H24 N5 06 S2 Zn
CI CCS, COM
SR CA
```

# Ring System Data

Elemental|Elemental| Size of |Ring System| Ring | RID Analysis |Sequence | the Rings| Formula |Identifier|Occurrence

### Page 85 -

ANSWER 4 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9

RN

ED

767616-38-6 REGISTRY
Entered STN: 24 Oct 2004
Zincate(1-), (butanoato-k0)(2-methyl-2-propanamine)bis(4(1H)-pyrimidinethionato-kS4)-, (T-4)- (9CI) (CA INDEX NAME) CN

C16 H24 N5 O2 S2 Zn MF

CCS, COM CI

CA SR

### Ring System Data

Elemental Analysis EA	Sequence	the Rings	Ring System Formula RF	Identifier	RID  Occurrence   Count
======== C4N2	+=======   NCNC3	+= <i>==</i> ====-   6	C4N2	46.195.23	2

L9

RN

ED

ANSWER 5 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN 765886-51-9 REGISTRY Entered STN: 20 Oct 2004 Zincate(1-), bis(2(3H)-benzothiazolethionato-kS2)(butanoato-kO)(2-propagazine) CN κ0)(2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

C21 H24 N3 O2 S4 Zn MF

CCS, COM CI SR

### Ring System Data

Analysis EA	Sequence   ES	the Rings	Ring System   Formula   RF	RID	RID Occurrence Count
	+=======   NCSC2-C6		+=======-   C7NS	333.521.13	2

ANSWER 6 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9

760160-39-2 REGISTRY RN

Entered STN: 11 Oct 2004 ED

Zincate(1-), bis(2(3H)-benzothiazolethionato-kS2)(butanoato-kO)(ethanamine)-, (T-4)- (9CI) (CA INDEX NAME)
C20 H22 N3 O2 S4 Zn CN

MF

CCS, COM CI

SR CA

Elemental	Elemental	Size of	Ring System	Taeutilier	RID
Analysis	Sequence	the Rings	Formula		Occurrence
EA	ES	SZ	RF		Count
========= C3NS-C6	-========   NCSC2-C6		c7NS	333.521.13	2

- ANSWER 7 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN 755740-20-6 REGISTRY L9
- RN
- ED
- Entered STN: 01 Oct 2004
  Zincate(1-), (butanoato-k0)(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-k52)-, (T-4)- (9CI) (CA INDEX NAME) CN
- C28 H34 N3 O2 S2 Zn MF

CCS, COM CICA SR

# Ring System Data

Analysis EA	Sequence   ES	the Rings	•	Identifier    RID	Count
======================================			+========-   C9N	591.79.43	2

L9 RN

ED

ANSWER 8 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN 750557-81-4 REGISTRY Entered STN: 24 Sep 2004 Zincate(1-), (butanoato-k0)(2-methyl-2-propanamine)bis(2(1H)-pyridinethionato-k52)-, (T-4)- (9CI) (CA INDEX NAME) C18 H26 N3 02 S2 Zn CN

MF

CCS, COM CI

SR CA

	Elemental	Size of	Ring System	Ring	RID
	Sequence	the Rings	Formula	Identifier	Occurrence
	ES	SZ	RF	RID	Count
======== C5N	+=======-   NC5	-====================================	C5N	46.156.21	2

L9 ANSWER 9 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 745776-79-8 REGISTRY
ED Entered STN: 16 Sep 2004
CN Zincate(2-), bis(methanamine)bis[sulfato(2-)-k0]-, (T-4)- (9CI) (CA INDEX NAME)
MF C2 H10 N2 O8 S2 Zn
CI CCS, COM
SR CA

ANSWER 10 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 742046-45-3 REGISTRY
ED Entered STN: 10 Sep 2004
CN Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-methyl-2-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
MF C22 H26 N3 O2 S4 Zn
CI CCS, COM
SR CA

EÁ	ES	SZ	Ring System Formula RF	RID	Count
======================================	•		+=======-   C7NS	333.521.13	2

```
L9 ANSWER 11 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 742042-77-9 REGISTRY
ED Entered STN: 10 Sep 2004
CN Cuprate(2-), bis(methanamine)bis[sulfato(2-)-k0]- (9CI) (CA INDEX NAME)
MF C2 H10 Cu N2 O8 S2
CI CCS, COM
SR CA
```

L9 ANSWER 12 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 740072-13-3 REGISTRY
ED Entered STN: 05 Sep 2004
CN Zincate(1-), (butanoato-κο)(2-methyl-2-propanamine)bis(2(1H)pyrazinethionato-κS2)-, (T-4)- (9CI) (CA INDEX NAME)
MF C16 H24 N5 02 S2 Zn
CI CCS, COM
SR CA

Elemental Analysis EA	ES	SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
======================================	:	+======-   6		-====================================	2

```
ANSWER 13 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     713079-80-2 REGISTRY
RN
     Entered STN: 20 Jul 2004
ED
     Cadmium, bis(4-aminobenzenesulfonato-κ0)tetrakis(1-propanamine)-,
CN
     (OC-6-12)-, compd. with 1-propanamine (1:1) (9CI) (CA INDEX NAME) C24 H48 Cd N6 O6 S2 . C3 H9 N
MF
SR
                 CA, CAPLUS
     STN Files:
LC
      CAplus document type: Journal
DT.CA
       Roles from non-patents: PREP (Preparation); PRP (Properties); RACT
RL.NP
       (Reactant or reagent)
```

# Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6   C	6 	C6	46.150.18	2 in CM  1

1  $\mathsf{CM}$ 

CRN 713079-79-9 CMF C24 H48 Cd N6 O6 S2 CCI CCS

# PAGE 1-A

# PAGE 2-A

2 CM

107-10-8 CRN CMF C3 H9 N

H3C-CH2-CH2-NH2

Experimental Property Tags (ETAG)

TROTERTT	NO	ΓΕ ====
Crystal Structure IR Absorption Spectra Molecular Structure		

Zhou, Jin-Sen; Dalton Transactions 2004(9) P1493-1497 CAPLUS (1)

See HELP PROPERTIES for information about property data sources in REGISTRY. 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

141:81204 CA AN Reversible and selective amine interactions of  $[Cd(\mu 2-N,0-p-$ TI NH2C6H4SO3)2(H2O)2]n Zhou, Jin-Sen; Cai, Jiwen; Wang, Li; Ng, Seik-Weng School of Chemistry & Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, Peop. Rep. China Dalton Transactions (2004), (9), 1493-1497 CODEN: DTARAF; ISSN: 1477-9226 ΑU

CS

S0

Royal Society of Chemistry

PB Journal DT

English LA

78-7 (Inorganic Chemicals and Reactions) CC

Section cross-reference(s): 75  $[Cd(\mu 2-N,0-p-NH2C6H4SO3)2(H2O)2]n$  (1) is a layered coordination compound The solid-vapor reactions between crystalline 1 and volatile amines were AB studied and the corresponding amine adducts were characterized by elemental anal., TGA, PXRD and IR. Among them, the C2H5NH2 and PrNH2 adducts, [Cd(C2H5NH2)4(H2O)2](H2NC6H4SO3)2 (3) and [Cd(PrNH2)4(O-p-H2NC6H4SO3)2] PrNH2 (4), grew into single crystals in situ from the solid-vapor reaction processes and their crystal structures were characterized. In both cases, 4 mol equivalent of amine mols. coordinate to Cd(II) via replacing the N,O-p-NH2C6H4SO3 ligands or coordinated H2O mols. The single-phase product suggests that the solid-vapor reaction between the metal sulfonate and volatile alkylamines could be used as a green process to synthesize monoamine-coordinated Cd(II) complexes without any solvent and routine separation Finally, the substitution reaction is reversible at room conditions and selective for primary alkylamines.

crystal structure cadmium alkylamine aminobenzenesulfonate; substitution layered cadmium aminobenzenesulfonate aqua complex alkylamine vapor ST reversible; cadmium alkylamine aminobenzenesulfonate prepn structure; sulfanilate cadmium aqua complex solid substitution alkylamine vapor

Amines, reactions IT RL: RCT (Reactant); RACT (Reactant or reagent)

```
(aliphatic; reversible solid-vapor coordinative substitution of layered
            cadmium(II) aminobenzenesulfonate aqua solid with volatile alkylamines)
       Crystal structure
IT
       Molecular structure
            (of layered cadmium(II) aminobenzenesulfonate aqua complex and
            alkylamine-substituted derivs.)
       Green chemistry
IT
       Substitution reaction, coordinative
            (reversible solid-vapor coordinative substitution of layered
            cadmium(II) aminobenzenesulfonate aqua solid with volatile alkylamines)
IT
       121-57-3
        RL: RCT (Reactant); RACT (Reactant or reagent)
             (for preparation of layered cadmium(II) aminobenzenesulfonate aqua complex
            and alkylamine-substituted derivs.)
       288855-36-7P
IT
        RL: SPN (Synthetic preparation); PREP (Preparation)
             (preparation from dehydration of layered cadmium(II) aminobenzenesulfonate
             aqua complex)
                               713079-80-2P
        713079-78-8P
IT
       RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
             (preparation via reversible solid-vapor coordinative substitution of layered
             cadmium(II) aminobenzenesulfonate aqua complex solid with volatile
       alkylamine, and crystal structure and TGA of)
74-89-5DP, Methylamine, reaction product with cadmium(II) sulfanilate aqua complex 75-31-0DP, Isopropylamine, reaction product with cadmium(II) sulfanilate aqua complex 75-64-9DP, tert-Butylamine, reaction product with cadmium(II) sulfanilate aqua complex 78-81-9DP, Isobutylamine,
IT
        with cadmium(II) sulfanilate aqua complex
        reaction product with cadmium(II) sulfanilate aqua_complex
                                                                                                        109-73-9DP,
        n-Butylamine, reaction product with cadmium(II) sulfanilate aqua complex
        713079-76-6DP, reaction products with alkylamines RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
        (Reactant or reagent)
             (preparation via solid-vapor coordinative substitution of layered solid with
             volatile alkylamine, and TGA of)
        713079-76-6P
IT
        RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
        (Preparation); RACT (Reactant or reagent)
        (preparation, layered crystal structure, dehydration, and reversible solid-vapor coordinative substitution with volatile alkylamines) 74-89-5, Methylamine, reactions 75-04-7, Ethylamine, reactions 75-33, Isopropylamine, reactions 75-64-9, tert-Butylamine, reactions 78-81-9, Isobutylamine 107-10-8, n-Propylamine, reactions 109-73-9, n-Putylamine 103-51-075
IT
        n-Butylamine, reactions
        RL: RCT (Reactant); RACT (Reactant or reagent) (reversible solid-vapor coordinative substitution of layered
             cadmium(II) aminobenzenesulfonate aqua complex solid with volatile
             alkylamine)
                      THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
(1) Albrecht, M; Angew Chem, Int Ed 2001, V40, P3750 CAPLUS (2) Albrecht, M; J Chem Soc, Dalton Trans 2000, P3797 CAPLUS
 (3) Albrecht, M; Nature 2000, V406, P970 CAPLUS
(3) Albrecht, M; Nature 2000, V406, P9/0 CAPLUS
(4) Braga, D; Chem Commun 2001, P2272 CAPLUS
(5) Braga, D; Organometallics 2002, V21, P1315 CAPLUS
(6) Buss, C; J Am Chem Soc 1998, V120, P7783 CAPLUS
(7) Buss, C; J Am Chem Soc 2002, V124, P1031 CAPLUS
(8) Cai, J; Acta Crystallogr, Sect B 2001, V57, P520 MEDLINE
(9) Cai, J; Chin J Inorg Chem 2003, V19, P81
(10) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(11) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(12) Cai, J; J Mater Chem 2003, V13, P1806 CAPLUS
 (12) Cai, J; J Mater Chem 2003, V13, P1806 CAPLUS
```

```
(13) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS (14) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS (15) Chandler, B; Chem Commun 2002, P1900 CAPLUS (16) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (17) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (17) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (17) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (17) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (17) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (17) Chem, C; Inorg Chem, C; Inor
 (17) Chen, C; J Chem Crystallogr 2001, V31, P271 CAPLUS
(17) Chen, C; J Chem Crystallogr 2001, V31, F271 CAPLUS
(18) Cote, A; Chem Commun 2001, P251 CAPLUS
(19) Cote, A; Coord Chem Rev 2003, V245, P49 CAPLUS
(20) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(21) Dalrymple, S; Chem Eur J 2002, V8, P3010 CAPLUS
(22) Drew, S; J Am Chem Soc 2001, V123, P8414 CAPLUS
(23) Fernandez, E; J Am Chem Soc 2003, V125, P2022 CAPLUS
(24) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
 (25) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(25) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(26) Kato, M; Angew Chem, Int Ed 2002, V41, P3183 CAPLUS
(27) Makinen, S; Chem Eur J 2001, V4, P5176
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Poppel, L; J Am Chem Soc 2003, V125, P11006
(30) Poppel, L; J Chem Soc, Dalton Trans 2002, P3327
(31) Shakeri, V; Z Kristallogr 1992, V198, P165 CAPLUS
(32) Sheldrick, G; SHELX97, Program for R-ray Crystal Structure Solution and Refinement 1997
(33) Shimizu G: Chem Mater 1998, V10, P3282 CAPLUS
  (33) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
 (34) Yu, J; Inorg Chem 2001, V40, P582 CAPLUS (35) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
  (36) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS
                           ANSWER 14 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
 L9
                           713079-79-9 REGISTRY
 RN
                           Entered STN: 20 Jul 2004
 ED
                          Cadmium, bis (4-aminobenzenesul fonato-\kappa 0) tetrakis (1-propanamine)-,
 CN
                            (OC-6-12)- (9CI) (CA INDEX NAME)
                            C24 H48 Cd N6 O6 S2
 MF
 CI
                           CCS, COM
 SR
```

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========= C6	+=======   C6	+========   6	C6	46.150.18	2

PAGE 2-A

 $H_3C-NH_2-Ni\frac{0}{-}PH_3$ 

# 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

140:357466 CA AN Theoretical studies on C-heteroatom bond formation via reductive TI elimination from group 10 M(PH3)2(CH3)(X) species (X = CH3, NH2, OH, SH) and the determination of metal-x bond strengths using density functional

MacGregor, Stuart A.; Neave, Greg W.; Smith, Christopher Department of Chemistry, School of Engineering and Physical Sciences, ΑU

Heriot-Watt University, Edinburgh, EH14 4AS, UK Faraday Discussions (2003), 124, 111-127 CODEN: FDISE6; ISSN: 1359-6640

**SO** 

Royal Society of Chemistry PB

Journal DT

LA English 29-13 (Organometallic and Organometalloidal Compounds) CC

Section cross-reference(s): 22

D. functional calcns. were used to investigate C-C, C-N and C-O bond forming reactions via reductive elimination from Group 10 cis-[M(PH3)2(Me)(X)] species (X = Me, NH2, OH). Both direct reaction from ΑB the four-coordinate species and a three-coordinate mechanism involving initial PH3 loss was considered. For the four-coordinate pathway the ease Initial PH3 loss was considered. For the Tour-coordinate pathway the ease of reductive elimination to give M(PH3)2 and Me-X follows the trend M = Pd < Pt < Ni. The reaction of the cis-M(PH3)2(Me)(NH2) species is promoted by the formation of methylamine adducts. Non-planar transition states are located and the C-heteroatom bond forming processes are characterized by migration of Me onto the cis-heteroatom ligand. For a given ligand, X, activation energies follow the trend M = Ni < Pd < Pt. Formation of the three-coordinate M(PH3)(Me)(X) species is promoted by a labilization of the cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OHthe cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OH. For the three-coordinate pathway the energy change for reductive elimination to give M(PH3) and Me-X again follows the trend M = Pd < Pt < PtNi and in all cases the initial product is an M(PH3)(XMe) adduct. three-coordinate transition states again involve migration of the Me ligand onto the cis-X ligand and for X = NH2 or OH activation energies follow the trend Ni > Pd < Pt. For a given metal activation energies in both the four- and three-coordinate pathways increase along the series Me < NH2 < OH. These trends in activation energy can be rationalized in terms of the strength of M-Me/M-X bonding as long as the extent of geometrical distortion required to obtain the transition state geometry is taken into account. Further calcns. on cis-Pd(PH3)2(Me)(SH) suggest that the more common exptl. observation of C(sp3)-S compared to C(sp3)-O reductive elimination arises from the greater kinetic accessibility of the former process rather than an intrinsic thermodn. preference for C-S bond formation. By comparison, the calcns. indicate that C(sp3)-N reductive elimination should be feasible from Ni and Pd systems. DF calcns. are shown to reproduce the relative homolytic bond strengths determined exptl. for Pt-X bonds. In the cis-M(PH3)2(Me)(X) systems the M-Me homolytic bond strength increases down the group while for M-NH2 and M-OH bonds the trend is  $M = Ni \approx Pd < Pt$ . M-NH2 and M-OH bonds are considerably stronger than M-Me bonds and the presence of a heteroatom ligand serves to weaken M-CH3 bonds even further.
nickel palladium platinum phosphine methyl complex reductive elimination

ST mechanism; Group 10 methyl alkoxy amido mercapto complex reductive elimination; reductive elimination DFT geometry Group 10 diphosphine methyl complex; activation energy DFT reductive elimination Group 10 methyl complex; transition state structure DFT reductive elimination methylnickel methylpalladium methylplatinum; mechanism four three

coordinate reductive elimination methylnickel methylpalladium methylplatinum Bond energy IT (DFT calcn. of homolytic bond strengths of Group 10 metals with carbon, nitrogen, oxygen an sulfur in reductive elimination from diphosphine complexes) Density functional theory IT Potential energy (DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Group VIII element complexes IT RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (Group 10; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) IT Bond formation (carbon-carbon, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Bond formation IT (carbon-nitrogen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Bond formation IT (carbon-oxygen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) **Bond formation** IT (carbon-sulfur; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Molecular structure IT (optimized; of nickel, palladium and platinum Me amido-, alkoxy- and mercapto-complexes) Activation energy IT Transition state structure (reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Elimination reaction, coordinative IT (reductive; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Coordination number IT (three; comparison of three- and four-coordinate pathway of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes by DFT geometry and energy profile calcn.) 682768-21-4, (Methanethiol)(phosphine)palladium IT RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) 682767-97-1, (Methanamine)bis(phosphine)nickel 682767-98-2, IT 682767-99-3, (Methanamine)bis(phosphine)palladium (Methanamine)bis(phosphine)platinum 682768-00-9. (Methanol)bis(phosphine)nickel RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (optimized geometry, potential energy, dissociation; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) 67-56-1, Methanol, properties 74-84-0, Ethane, properties IT

```
Methanamine, properties 66048-71-3, Bis(phosphine)nickel 76830-85-8 Bis(phosphine)platinum 78452-79-6, Bis(phosphine)palladium 682768-1682768-11-2 682768-12-3 682768-13-4, (Methanamine)(phosphine)nickel 682768-14-5, (Methanamine)(phosphine)palladium 682768-15-6, (Methanamine)(phosphine)palladium 682768-15-6,
                                                                                                                                 76830-85-8
                                                                                                                                     682768-10-1
                                                                             682768-16-7
          (Methanamine)(phosphine)platinum
                                                                    682768-17-8, (Methanol)(phosphine)palladium
          (Methanol)(phosphine)nickel
         682768-18-9, (Methanol)(phosphine)platinum (Methanethiol)bis(phosphine)palladium
                                                                                                  682768-20-3.
         RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
         nonpreparative)
                (optimized geometry, potential energy; DFT geometry and energy profile
               of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
               mercapto-complexes)
         79218-09-0, Dimethyl(phosphine)palladium
         Dimethyl (phosphine) nickel 682768-03-2, Dimethyl (phosphine) platinum 682768-04-3, (Amido) (methyl) (phosphine) nickel 682768-05-4, (Amido) (methyl) (phosphine) nickel 682768-05-4,
                                                                                              682768-02-1.
IT
         b82/b8-U4-3, (Amido)(metnyl)(phosphine)nickel b82/b8-U5-4, (Amido)(methyl)(phosphine)palladium 682768-06-5, (Amido)(methyl)(phosphine)platinum 682768-07-6, (Hydroxo)(methyl)(phosphine)nickel 682768-08-7, (Hydroxo)(methyl)(phosphine)palladium 682768-09-8, (Hydroxo)(methyl)(phosphine)platinum 682768-19-0 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
                (optimized geometry, potential energy; DFT geometry and energy profile
               of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
                mercapto-complexes)
                                   79218-07-8
                                                                                       682767-91-5
                                                             79232-18-1
          79218-06-7
IT
                                                                                        682767-92-6
          cis-(Amido)methylbis(phosphine)nickel
                                                                                               682767-93-7,
          cis-(Amido)methylbis(phosphine)palladium
                                                                                             682767-94-8,
          cis-(Amido)methylbis(phosphine)platinum
         cis-(Hydroxo)methylbis(phosphine)nickel 6cis-(Hydroxo)methylbis(phosphine)palladium
                                                                                             682767-95-9
                                                                                                   682767-96-0,
          cis-(Hydroxo)methylbis(phosphine)platinum
                                                                                                 682768-01-0
          RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
                (optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
                mercapto-complexes)
                            THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Albright, T; Orbital Interactions in Chemistry 1985
(1) Albright, I; Urbital Interactions in Chemistry 1985
(2) Ananikov, V; J Am Chem Soc 2002, V124, P2839 CAPLUS
(3) Baerends, E; Chem Phys 1973, V2, P41 CAPLUS
(4) Becke, A; Phys Rev A 1988, V38, P3098 CAPLUS
(5) Bernard, K; Organometallics 1989, V8, P795 CAPLUS
(6) Blomberg, M; J Am Chem Soc 1991, V113, P424 CAPLUS
(7) Bryndza, H; J Am Chem Soc 1987, V109, P1444 CAPLUS
(8) Bryndza, H; Organometallics 1984, V3, P1603 CAPLUS
(9) Carpita, A; Tetrahedron Lett 1989, V30, P2699 CAPLUS
(10) Christau, H: Synthesis 1981, P892
(10) Christau, H; Synthesis 1981, P892
(11) Collman, J; Principles and Applications of Organotransition Metal
        Chemistry 1987
(12) Crabtree, R; The Organometallic Chemistry of the Transition Metals 1988
(12) Craptree, K; The Organometallic Chemistry of the Transii (13) Dedieu, A; Chem Rev 2000, V100, P543 CAPLUS (14) Dunbar, K; Inorg Chim Acta 1995, V240, P527 CAPLUS (15) Empsall, H; J Chem Soc, Dalton Trans 1974, P1980 CAPLUS (16) Fan, L; J Am Chem Soc 1992, V114, P10890 CAPLUS (17) Fan, L; J Chem Phys 1992, V96, P6937 CAPLUS (18) Fan, L; J Chem Phys 1992, V96, P9005 CAPLUS (19) Fulton, J; Acc Chem Res 2002, V35, P44 CAPLUS (20) Guerra C: Theor Chem Acc 1998, V99, P301 CAPLUS
(20) Guerra, C; Theor Chem Acc 1998, V99, P391 CAPLUS (21) Haar, C; Organometallics 1999, V18, P474 CAPLUS
(22) Haarman, H; Inorg Chim Acta 1998, V270, P34 CAPLUS
```

```
(23) Han, R; J Am Chem Soc 1997, V119, P8135 CAPLUS (24) Han, R; J Am Chem Soc 1998, V120, P7657 CAPLUS
(25) Hartwig, J; Acc Chem Res 1998, V31, P852 CAPLUS (26) Hartwig, J; Angew Chem, Int Ed Engl 1998, V37, P2047 (27) Hartwig, J; Pure Appl Chem 1999, V8, P1417
(27) Hartwig, J, Pure Appl Chem 1933, vo, F1717
(28) Hartwig, J; Synlett 1997, P329 CAPLUS
(29) Ittel, S; J Am Chem Soc 1978, V100, P7577 CAPLUS
(30) Jones, C; J Chem Soc, Dalton Trans 1974, P992 CAPLUS
(31) Komiya, S; Organometallics 1985, V4, P1130 CAPLUS
(32) Koo, K; Organometallics 1996, V15, P2669 CAPLUS
(33) Koo, K; Organometallics 1998, V17, P2924 CAPLUS
(34) Kosugi M: Rull Chem Soc Inn 1985, V58, P3657 CAPLUS
 (34) Kosugi, M; Bull Chem Soc Jpn 1985, V58, P3657 CAPLUS
(35) Kosugi, M; Chem Lett 1983, P927 CAPLUS
(36) Lin, B; J Am Chem Soc 2002, V124, P2890 CAPLUS
(37) Low, J; J Am Chem Soc 1986, V108, P6115 CAPLUS
 (38) Low, J; Organometallics 1986, V5, P609 CAPLUS
(39) Macgregor, S; Inorg Chem 1999, V38, P4868 CAPLUS
(40) Macgregor, S; Organometallics 2001, V20, P1860 CAPLUS
(41) Mann, G; J Am Chem Soc 1996, V118, P13109 CAPLUS
(42) Mann, G; J Am Chem Soc 1998, V120, P9205 CAPLUS
(42) Mann, G; J Am Chem Soc 1998, V120, P9205 CAPLUS
(43) Matsubara, T; Organometallics 2002, V21, P2662 CAPLUS
(44) Matsubara, T; Organometallics 2002, V21, P4482 CAPLUS
(45) Matsunaga, P; Polyhedron 1995, V14, P175 CAPLUS
(46) Muri, A; Top Curr Chem 2002, V219, P131
(47) Niu, S; Chem Rev 2000, V100, P353 CAPLUS
(48) Perdew, J; Phys Rev B 1986, V33, P8822
(49) Poignant, G; Organometallics 1997, V16, P124 CAPLUS
(50) Sakaki, S; Inorg Chem 1994, V33, P1660 CAPLUS
(51) Sakaki, S; J Am Chem Soc 1993, V115, P2373 CAPLUS
 (51) Sakaki, S; J Am Chem Soc 1993, V115, P2373 CAPLUS
 (52) Sakaki, S; J Organomet Chem 2000, V611, P288 CAPLUS
(52) Sakaki, S; J Organomet Chem 2000, V611, P288 CAPLUS
(53) Sakaki, S; J Phys Chem A 1998, V102, P8027 CAPLUS
(54) Sakaki, S; Organometallics 1999, V18, P4825 CAPLUS
(55) Siegbahn, P; J Am Chem Soc 1992, V114, P10548 CAPLUS
(56) Snijders, J; Mol Phys 1979, V38, P1909 CAPLUS
(57) Stille, J; The Chemistry of the Metal-Carbon Bond 1985, V2 CAPLUS
(58) Takagi, K; Chem Lett 1987, P2221 CAPLUS
(59) Tatsumi, K; Bull Chem Soc Jpn 1981, V54, P1857 CAPLUS
(60) Ta Velda G: J Comput Phys 1992, V99, P84 CAPLUS
 (60) Te Velde, G; J Comput Phys 1992, V99, P84 CAPLUS
(61) Thompson, J; Organometallics 1991, V10, P3906 CAPLUS
(62) Tolman, C; J Am Chem Soc 1979, V101, P1742 CAPLUS
(63) Torrent, M; Organometallics 2000, V19, P4402 CAPLUS
(64) van Lenthe, E; J Chem Phys 1993, V99, P4597 CAPLUS
(65) van der Boom, M; Angew Chem Int Ed Engl 1997, V36, P625 CAPLUS
(66) van der Boom, M; J Am Chem Soc 1998, V120, P6531 CAPLUS
(67) Versluis J: Chem Phys 1988 V88 P322 CAPLUS
 (67) Versluis, L; Chem Phys 1988, V88, P322 CAPLUS
(68) Villanueva, L; Organometallics 1994, V13, P3921 CAPLUS
(69) Weast, R; CRC Handbook of Chemistry and Physics, 60th edn 1981
  (70) Williams, B; J Am Chem Soc 1999, V121, P252 CAPLUS
 (71) Williams, B; J Am Chem Soc 2001, V123, P2576 CAPLUS (72) Wolfe, J; Acc Chem Res 1998, V31, P805 CAPLUS
 (73) Yang, B; J Organomet Chem 1999, V576, P125 CAPLUS (74) Ziegler, T; J Phys Chem 1989, V93, P3050 CAPLUS
               ANSWER 16 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN 682767-97-1 REGISTRY Entered STN: 18 May 2004
 L9
 RN
 ED
                Nickel, (methanamine)bis(phosphine)- (9CI) (CA INDEX NAME)
 OTHER NAMES:
                (Methanamine)bis(phosphine)nickel
 CN
                C H11 N Ni P2
 MF
 CI
                CCS
```

SR STN Files: CA, CAPLUS LC DT.CA CAplus document type: Journal RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PRP (Properties); RACT (Reactant or reagent)

PH<sub>3</sub> H<sub>3</sub>P-Ni 0 NH<sub>2</sub>-CH<sub>3</sub>

> 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

140:357466 CA AN Theoretical studies on C-heteroatom bond formation via reductive TI elimination from group 10 M(PH3)2(CH3)(X) species (X = CH3, NH2, OH, SH) and the determination of metal-X bond strengths using density functional theory

MacGregor, Stuart A.; Neave, Greg W.; Smith, Christopher Department of Chemistry, School of Engineering and Physical Sciences, CS

Heriot-Watt University, Edinburgh, EH14 4AS, UK Faraday Discussions (2003), 124, 111-127 CODEN: FDISE6; ISSN: 1359-6640

SO

Royal Society of Chemistry PB

DT Journal English LA

AB

29-13 (Organometallic and Organometalloidal Compounds) CC

Section cross-reference(s): 22 D. functional calcns. were used to investigate C-C, C-N and C-O bond forming reactions via reductive elimination from Group 10 cis-[M(PH3)2(Me)(X)] species (X = Me, NH2, OH). Both direct reaction from the four-coordinate species and a three-coordinate mechanism involving the tour-coordinate species and a three-coordinate mechanism involving initial PH3 loss was considered. For the four-coordinate pathway the ease of reductive elimination to give M(PH3)2 and Me-X follows the trend M = Pd < Pt < Ni. The reaction of the cis-M(PH3)2(Me)(NH2) species is promoted by the formation of methylamine adducts. Non-planar transition states are located and the C-heteroatom bond forming processes are characterized by migration of Me onto the cis-heteroatom ligand. For a given ligand, X, activation energies follow the trend M = Ni < Pd < Pt. Formation of the three-coordinate M(PH3)(Me)(X) species is promoted by a labilization of the cis-PH3 ligand in the four-coordinate reactants when X = NH2 or OH. For the three-coordinate pathway the energy change for reductive elimination to give M(PH3) and Me-X again follows the trend M = Pd < Pt <Ni and in all cases the initial product is an M(PH3)(XMe) adduct. three-coordinate transition states again involve migration of the Me ligand onto the cis-X ligand and for X = NH2 or OH activation energies follow the trend Ni > Pd < Pt. For a given metal activation energies in both the four- and three-coordinate pathways increase along the series Me < NH2 < OH. These trends in activation energy can be rationalized in terms of the strength of M-Me/M-X bonding as long as the extent of geometrical distortion required to obtain the transition state geometry is taken into account. Further calcns. on cis-Pd(PH3)2(Me)(SH) suggest that the more common exptl. observation of C(sp3)-S compared to C(sp3)-O reductive elimination arises from the greater kinetic accessibility of the former process rather than an intrinsic thermodn. preference for C-S bond formation. By comparison, the calcns. indicate that C(sp3)-N reductive elimination should be feasible from Ni and Pd systems. DF calcns. are

shown to reproduce the relative homolytic bond strengths determined exptl. for Pt-X bonds. In the cis-M(PH3)2(Me)(X) systems the M-Me homolytic bond strength increases down the group while for M-NH2 and M-OH bonds the trend is M = Ni  $\approx$  Pd < Pt. M-NH2 and M-OH bonds are considerably stronger than M-Me bonds and the presence of a heteroatom ligand serves to weaken M-CH3 bonds even further. nickel palladium platinum phosphine methyl complex reductive elimination ST mechanism; Group 10 methyl alkoxy amido mercapto complex reductive elimination; reductive elimination DFT geometry Group 10 diphosphine methyl complex; activation energy DFT reductive elimination Group 10 methyl complex; transition state structure DFT reductive elimination methýlnickel methylpalladium methylplatinum; mechanism four three coordinate reductive elimination methylnickel methylpalladium methylplatinum Bond energy IT (DFT calcn. of homolytic bond strengths of Group 10 metals with carbon, nitrogen, oxygen an sulfur in reductive elimination from diphosphine complexes) Density functional theory IT Potential energy (DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes)
Group VIII element complexes IT RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(Group 10; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Bond formation IT (carbon-carbon, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Bond formation IT (carbon-nitrogen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) **Bond formation** IT (carbon-oxygen, reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) IT Bond formation (carbon-sulfur; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Molecular structure IT (optimized; of nickel, palladium and platinum Me amido-, alkoxy- and mercapto-complexes) Activation energy IT Transition state structure (reductive elimination; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Elimination reaction, coordinative IT (reductive; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) Coordination number IT (three; comparison of three- and four-coordinate pathway of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes by DFT geometry and energy profile calcn.) 682768-21-4, (Methanethiol)(phosphine)palladium IT RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

```
(DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and mercapto-complexes) 682767-97-1, (Methanamine)bis(phosphine)nickel 682767-98-2, (Methanamine)bis(phosphine)palladium 682767-99-3,
IT
                                                                         682768-00-9.
         (Methanamine)bis(phosphine)platinum
         (Methanol)bis(phosphine)nickel
        RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (optimized geometry, potential energy, dissociation; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me
        amido-, alkoxy- and mercapto-complexes) 67-56-1, Methanol, properties 74-84-0, E
                                                   rties 74-84-0, Ethane, properties
66048-71-3, Bis(phosphine)nickel
78452-79-6, Bis(phosphine)palladium
                                                                                                                   74-89-5,
IT
                                                                                                                 76830-85-8
        Methanamine, properties
                                                                                                                    682768-10-1
        Bis(phosphine)platinum
                                                        682768-13-4, (Methanamine) (phosphine) nickel
                                682768-12-3
        682768-11-2
        682768-14-5, (Methanamine)(phosphine)palladium
                                                                                            682768-15-6,
         (Methanamine)(phosphine)platinum
                                                                    682768-16-7,
                                                            682768-17-8, (Methanol)(phosphine)palladium
         (Methanol)(phosphine)nickel
        682768-18-9, (Methanol)(phosphine)platinum
                                                                                     682.768-20-3, . .
        (Methanethiol)bis(phosphine)palladium RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation,
         nonpreparative)
             (optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
              mercapto-complexes)
        79218-09-0, Dimethyl(phosphine)palladium
                                                                                  682768-02-1,
IT
                                                        682768-03-2, Dimethyl(phosphine)platinum
         Dimethyl(phosphine)nickel
        682768-04-3, (Amido) (methyl) (phosphine) nickel (Amido) (methyl) (phosphine) palladium 682768-
                                                                                           682768-05-4.
                                                                          682768-06-5.
                                                                        682768-07-6,
         (Amido)(methyl)(phosphine)platinum
                                                                        682768-08-7,

682768-09-8,

682768-19-0
         (Hydroxo)(methyl)(phosphine)nickel
         (Hydroxo) (methyl) (phosphine) palladium
         (Hydroxo) (methyl) (phosphine) platinum
        RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent) (optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
              mercapto-complexes)
                              79218-07-8
                                                                            682767-91-5,
         79218-06-7
                                                     79232-18-1
IŤ
                                                                             682767-92-6
         cis-(Amido)methylbis(phosphine)nickel
         cis-(Amido)methylbis(phosphine)palladium
                                                                                   682767-93-7,
                                                                                 682767-94-8,
682767-95-9,
         cis-(Amido)methylbis(phosphine)platinum
        cis-(Hydroxo)methylbis(phosphine)nickel 6
cis-(Hydroxo)methylbis(phosphine)palladium
cis-(Hydroxo)methylbis(phosphine)platinum
                                                                                      682767-96-0.
                                                                                    682768-01-0
        RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (optimized geometry, potential energy; DFT geometry and energy profile of reductive elimination of Group 10 dimethyl-, Me amido-, alkoxy- and
              mercapto-complexes)
                        THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Albright, T; Orbital Interactions in Chemistry 1985
(2) Ananikov, V; J Am Chem Soc 2002, V124, P2839 CAPLUS
(3) Baerends, E; Chem Phys 1973, V2, P41 CAPLUS
(4) Becke, A; Phys Rev A 1988, V38, P3098 CAPLUS
(5) Bernard, K; Organometallics 1989, V8, P795 CAPLUS
(6) Blomberg, M; J Am Chem Soc 1991, V113, P424 CAPLUS
(7) Bryndza, H; J Am Chem Soc 1987, V109, P1444 CAPLUS
(8) Bryndza, H; Organometallics 1984, V3, P1603 CAPLUS
(9) Carpita, A; Tetrahedron Lett 1989, V30, P2699 CAPLUS
 (10) Christau, H; Synthesis 1981, P892
(11) Collman, J; Principles and Applications of Organotransition Metal
```

```
Chemistry 1987
 (12) Crabtree, R; The Organometallic Chemistry of the Transition Metals 1988
 (13) Dedieu, A; Chem Rev 2000, V100, P543 CAPLUS
(14) Dunbar, K; Inorg Chim Acta 1995, V240, P527 CAPLUS
(14) Dunbar, K; Inorg Chim Acta 1995, V240, P52/ CAPLUS
(15) Empsall, H; J Chem Soc, Dalton Trans 1974, P1980 CAPLUS
(16) Fan, L; J Am Chem Soc 1992, V114, P10890 CAPLUS
(17) Fan, L; J Chem Phys 1992, V96, P6937 CAPLUS
(18) Fan, L; J Chem Phys 1992, V96, P9005 CAPLUS
(19) Fulton, J; Acc Chem Res 2002, V35, P44 CAPLUS
(20) Guerra, C; Theor Chem Acc 1998, V99, P391 CAPLUS
(21) Haar, C; Organometallics 1999, V18, P474 CAPLUS
(22) Haarman, H: Thorg Chim Acta 1998, V270, P34 CAPLUS
 (22) Haarman, H; Inorg Chim Acta 1998, V270, P34 CAPLUS
(23) Han, R; J Am Chem Soc 1997, V119, P8135 CAPLUS
(24) Han, R; J Am Chem Soc 1998, V120, P7657 CAPLUS
(25) Hartwig, J; Acc Chem Res 1998, V31, P852 CAPLUS
(26) Hartwig, J; Angew Chem, Int Ed Engl 1998, V37, P2047
(27) Hartwig, J; Pure Appl Chem 1999, V8, P1417
(27) Hartwig, J; Pure Appl Chem 1999, V8, P1417
(28) Hartwig, J; Synlett 1997, P329 CAPLUS
(29) Ittel, S; J Am Chem Soc 1978, V100, P7577 CAPLUS
(30) Jones, C; J Chem Soc, Dalton Trans 1974, P992 CAPLUS
(31) Komiya, S; Organometallics 1985, V4, P1130 CAPLUS
(32) Koo, K; Organometallics 1996, V15, P2669 CAPLUS
(33) Koo, K; Organometallics 1998, V17, P2924 CAPLUS
(34) Kosugi, M; Bull Chem Soc Jpn 1985, V58, P3657 CAPLUS
(35) Kosugi, M; Chem Lett 1983, P927 CAPLUS
(36) Lin, B; J Am Chem Soc 2002, V124, P2890 CAPLUS
(37) Low, J; J Am Chem Soc 1986, V108, P6115 CAPLUS
(38) Low, J: Organometallics 1986, V5, P609 CAPLUS
 (37) Low, J; J Am Chem Soc 1986, V108, P6115 CAPLUS
(38) Low, J; Organometallics 1986, V5, P609 CAPLUS
(39) Macgregor, S; Inorg Chem 1999, V38, P4868 CAPLUS
(40) Macgregor, S; Organometallics 2001, V20, P1860 CAPLUS
(41) Mann, G; J Am Chem Soc 1996, V118, P13109 CAPLUS
(42) Mann, G; J Am Chem Soc 1998, V120, P9205 CAPLUS
(43) Matsubara, T; Organometallics 2002, V21, P2662 CAPLUS
(44) Matsubara, T; Organometallics 2002, V21, P4482 CAPLUS
(45) Matsunaga, P; Polyhedron 1995, V14, P175 CAPLUS
(46) Muri, A; Top Curr Chem 2002, V219, P131
(47) Niu, S; Chem Rev 2000, V100, P353 CAPLUS
(48) Perdew, J; Phys Rev B 1986, V33, P8822
(49) Poignant, G; Organometallics 1997, V16, P124 CAPLUS
   (49) Poignant, G; Organometallics 1997, V16, P124 CAPLUS
   (50) Sakaki, Ś; Inorg Chem 1994, V33, P1660 CAPLUS
 (50) Sakaki, S; Inorg Chem 1994, V33, P1660 CAPLUS
(51) Sakaki, S; J Am Chem Soc 1993, V115, P2373 CAPLUS
(52) Sakaki, S; J Organomet Chem 2000, V611, P288 CAPLUS
(53) Sakaki, S; J Phys Chem A 1998, V102, P8027 CAPLUS
(54) Sakaki, S; Organometallics 1999, V18, P4825 CAPLUS
(55) Siegbahn, P; J Am Chem Soc 1992, V114, P10548 CAPLUS
(56) Snijders, J; Mol Phys 1979, V38, P1909 CAPLUS
(57) Stille, J; The Chemistry of the Metal-Carbon Bond 1985, V2 CAPLUS
(58) Takagi, K; Chem Lett 1987, P2221 CAPLUS
(59) Tatsumi, K; Bull Chem Soc Jpn 1981, V54, P1857 CAPLUS
(60) Te Velde. G: J Comput Phys 1992, V99, P84 CAPLUS
   (60) Te Velde, G; J Comput Phys 1992, V99, P84 CAPLUS
 (60) Te Velde, G; J Comput Phys 1992, V99, P84 CAPLUS
(61) Thompson, J; Organometallics 1991, V10, P3906 CAPLUS
(62) Tolman, C; J Am Chem Soc 1979, V101, P1742 CAPLUS
(63) Torrent, M; Organometallics 2000, V19, P4402 CAPLUS
(64) van Lenthe, E; J Chem Phys 1993, V99, P4597 CAPLUS
(65) van der Boom, M; Angew Chem Int Ed Engl 1997, V36, P625 CAPLUS
(66) van der Boom, M; J Am Chem Soc 1998, V120, P6531 CAPLUS
(67) Versluis, L; Chem Phys 1988, V88, P322 CAPLUS
(68) Villanueva, L; Organometallics 1994, V13, P3921 CAPLUS
(69) Weast, R; CRC Handbook of Chemistry and Physics, 60th edn 1981
(70) Williams, B; J Am Chem Soc 1999, V121, P252 CAPLUS
     (70) Williams, B; J Am Chem Soc 1999, V121, P252 CAPLUS
   (71) Williams, B; J Am Chem Soc 2001, V123, P2576 CAPLUS
```

(72) Wolfe, J; Acc Chem Res 1998, V31, P805 CAPLUS (73) Yang, B; J Organomet Chem 1999, V576, P125 CAPLUS (74) Ziegler, T; J Phys Chem 1989, V93, P3050 CAPLUS ANSWER 17 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN L9 595548-20-2 REGISTRY Entered STN: 30 Sep 2003 RN Cadmium, bis(2-methyl-1-propanamine)[1,5-naphthalenedisulfonato(2-)- $\kappa$ O]-, compd. with 2-methyl-1-propanamine (1:1), dihydrate (9CI) (CA ED CN INDEX NAME) C18 H28 Cd N2 O6 S2 . C4 H11 N . 2 H2 O MF SR STN Files: CA, CAPLUS LC DT.CA CAplus document type: Journal Roles from non-patents: PREP (Preparation); PRP (Properties); RACT RL.NP (Reactant or reagent)

### Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
c6-c6	-====================================	-========  6-6 	C10	591.49.57	1 in CM

CM 1 CRN 595548-19-9 CMF C18 H28 Cd N2 O6 S2

NH2-Bu-i

CCI CCS

2 CM

CRN 78-81-9 CMF C4 H11 N

Experimental Property Tags (ETAG)

PROPERTY	NO	
	(1)	CAS

Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811 (1)

See HELP PROPERTIES for information about property data sources in REGISTRY. 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

139:239001 CA AN Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2] TI Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang school of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China Journal of Materials Chemistry (2003), 13(7), 1806-1811 ΑU CS SO CODEN: JMACEP; ISSN: 0959-9428 Royal Society of Chemistry PB Journal DT English

LA

78-3 (Inorganic Chemicals and Reactions) CC [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. AB without dehydration and form stable adducts, via solid-vapor reaction at room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material. cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation

ST Thermal decomposition IT

(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)

IT

Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent) (primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

Intercalation IT (selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

595548-14-4P 595548-16-6P 595548-10-0P 595548-12-2P 595548-08-6P 595548-21-3P 595548-22-4P 595548-20-2P 595548-18-8P RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)

473251-23-9P IT

IT

```
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
          (Preparation); RACT (Reactant or reagent)
                 (preparation, thermal decomposition and selective amine coordinative
                substitution/intercalation behavior of cadmium diaqua
                naphthalenedisulfonate complex)
          81-04-9, 1,5-Naphthalenedisulfonic acid
IT
         RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
                           THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS (4) Cai, J; Unpublished results (5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS (6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS (7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS (8) Chen, C; J Chem Compatibility 2001, V2, P271
(/) Chen, C; Inorg Chem 2002, V41, P496/ CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dver A: An Introduction to Zeolite Molecular Sieves
(14) Cussen, E, J Am Chem Soc 2002, V124, P95/4 CAPLUS
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
(16) Eddoudi, M; Acc Chem Res 2001, V34, P319
(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li Nature 1999, V402, P276 CAPLUS
 (21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Commun 2003, P854 CAPLUS
                       ; J Am Chem Soc 2003, V125, P3062 CAPLUS
 (27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
 (28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS (29) Querler, L; C R Acad Sci Ser C 1972, V275, P321 (30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS (31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
 (32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS (34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS (35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS
          ANSWER 18 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
          595548-19-9 REGISTRY
Entered STN: 30 Sep 2003
RN
ED
          Cadmium, bis(2-methyl-1-propanamine)[1,5-naphthalenedisulfonato(2-)-
 CN
           κ0]- (9CI) (CA INDEX NAME)
          C18 H28 Cd N2 O6 S2
MF
           CCS, COM
CI
 SR
           CA
 Ring System Data
 Elemental|Elemental| Size of |Ring System|
                                                                                            Rina
                                                                                   |Identifier|Occurrence
 Analysis |Sequence |the Rings| Formula
                                                                                                          Count
                                                                                            RID
                                               SZ
                                                                     RF
       EA
                           ES
                                                                               ===+==================
                                                                                    |591.49.57 |1
                                       16-6
                                                            |C10
                   1c6-c6
```

C6-C6

Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
c6-c6	+=======  C6-C6 	6-6	c10	591.49.57	1 in CM 1

CM 1

CRN 595548-17-7

CMF C18 H28 Cd N2 06 S2

CCI CCS

(Reactant or reagent)

CM 2 CRN 109-73-9 Page 107-1

CMF C4 H11 N

H3C-CH2-CH2-CH2-NH2

Experimental Property Tags (ETAG)

INOILNI	NOTE	
IR Spectra X-Ray Diffraction Pattern	(1) (1)	CAS CAS

Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811 (1) **CAPLUS** 

See HELP PROPERTIES for information about property data sources in REGISTRY. 1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

139:239001 CA AN Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2] TI

Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang ΑU

School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) University, Canton, 510275, Peop. Rep. China Journal of Materials Chemistry (2003), 13(7), 1806-1811 CS

S<sub>0</sub> CODEN: JMACEP; ISSN: 0959-9428

Royal Society of Chemistry PB

Journal DT English LA

78-3 (Inorganic Chemicals and Reactions)

CC [Cd(1,5-nds)(H20)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered AB metal sulfonate. It can selectively intercalate ammonia and amines quant. metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature. The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed. The intercalation process is reversible, selective and preferential, indicating that the title compound reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.

cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation ST

Thermal decomposition TT

(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)

Amines, reactions IT

RL: RCT (Reactant); RACT (Reactant or reagent) (primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

Intercalation IT (selective amine coordinative substitution/intercalation behavior of

```
cadmium diaqua naphthalenedisulfonate complex)
                                                                                                                     595548-16-6P
                                                                                          595548-14-4P
                                                               595548-12-2P
                                    595548-10-0P
         595548-08-6P
IT
                                                                                          595548-22-4P
                                                               595548-21-3P
                                    595548-20-2P
         595548-18-8P
        RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
         (Preparation); RACT (Reactant or reagent)
              (preparation and thermal decomposition by selective amine coordinative
              substitution/intercalation of cadmium diaqua naphthalenedisulfonate
              complex)
        473251-23-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
IT
               (preparation, thermal decomposition and selective amine coordinative
              substitution/intercalation behavior of cadmium diaqua
              naphthalenedisulfonate complex)
         81-04-9, 1,5-Naphthalenedisulfonic acid
IT
         RL: RCT (Reactant); RACT (Reactant or reagent)
               (reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
                         THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973 (11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS (12) Cote, A; Chem Commun 2001, P251 CAPLUS (13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS (14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS (15) Page A; An Introduction to Zeolite Molecular Sieves
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
 (16) Eddoudi, M; Acc Chem Res 2001, V34, P319
 (17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS
(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Commun 2003, P854 CAPLUS
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Panaefstathiou G: Angew Chem Int Ed 2002, V41 P20
 (27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS (28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
 (29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
 (30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS (31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
 (32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS (34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS (35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS
         ANSWER 20 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN 595548-17-7 REGISTRY Entered STN: 30 Sep 2003
L9
RN
ED
         Cadmium, bis(1-butanamine)[1,5-naphthalenedisulfonato(2-)-KO]- (9CI)
CN
          (CA INDEX NAME)
          C18 H28 Cd N2 O6 S2
MF
          CCS, COM
CI
```

#### CA SR

# Ring System Data

EA	ES	SZ	, ,,,	I KID	RID Occurrence Count
	=+=======  C6-C6		+========  C10	591.49.57	1

```
ANSWER 21 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
          595548-16-6 REGISTRY
Entered STN: 30 Sep 2003
Cadmium, [1,5-naphthalenedisulfonato(2-)-κ0]bis(2-propanamine)-,
compd. with 2-propanamine (1:1), dihydrate (9CI) (CA INDEX NAME)
C16 H24 Cd N2 O6 S2 . C3 H9 N . 2 H2 O
RN
ED
```

CN

MF

SR

STN Files: CA, CAPLUS LC

DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

### Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
c6-c6	+======-  C6-C6 	-====================================	C10 	591.49.57	1 in CM

CM 1

CRN 595548-15-5

CMF C16 H24 Cd N2 O6 S2

CCI CCS

2 CM

CRN 75-31-0 CMF C3 H9 N

NH<sub>2</sub> H3C-CH-CH3

Experimental Property Tags (ETAG)

NOTE PROPERTY (1) CAS IR Spectra X-Ray Diffraction Pattern (1) CAS

Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811 (1)CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY. 1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

139:239001 CA

ΑN Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2] TI Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) ΑU CS University, Canton, 510275, Peop. Rep. China Journal of Materials Chemistry (2003), 13(7), 1806-1811 \$0 CODEN: JMACEP; ISSN: 0959-9428 Royal Society of Chemistry PB DT Journal English LA

78-3 (Inorganic Chemicals and Reactions) CC [Cd(1,5-nds)(H20)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered AB metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature. The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PRH2. TGA-IR analyses show that amines were

```
intercalated by interactions of different nature. Of these, 2 M amts. of
        amine mols. were intercalated by coordinative bonds replacing the
        coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is
        reversible, selective and preferential, indicating that the title compound
        could be designed as an amine-sensitive material.
cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
ST
         Thermal decomposition
IT
               (of cadmium naphthalenedisulfonate with coordinated/intercalated
               amines)
         Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
IT
               (primary; selective amine coordinative substitution/intercalation
               behavior of cadmium diaqua naphthalenedisulfonate complex)
         Intercalation
IT
               (selective amine coordinative substitution/intercalation behavior of
               cadmium diaqua naphthalenedisulfonate complex)
                                                                                                                          595548-16-6P
                                                                  595548-12-2P
                                                                                             595548-14-4P
                                     595548-10-0P
         595548-08-6P
IT
                                                                  595548-21-3P
                                                                                           . 595548-22-4P
                                     595548-20-2P
         595548-18-8P
         RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and thermal decomposition by selective amine coordinative
               substitution/intercalation of cadmium diaqua naphthalenedisulfonate
               complex)
         473251-23-9P
IT
         RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
          (Preparation); RACT (Reactant or reagent)
               (preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua
         naphthalenedisulfonate complex)
81-04-9, 1,5-Naphthalenedisulfonic acid
IT
         RL: RCT (Reactant); RACT (Reactant or reagent)
                (reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
                          THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dver. A: An Introduction to Zeolite Molecular Sieves 1
 (15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
 (16) Eddoudi, M; Acc Chem Res 2001, V34, P319
(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS

(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS

(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS

(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS

(21) Li, H; Nature 1999, V402, P276 CAPLUS

(22) Makinen, S; Chem Eur J 2001, V4, P5176

(23) Min K; J Am Chem Soc 2000, V122, P6834 CAPLUS
 (23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS (24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS (25) Pan, L; Chem Commun 2003, P854 CAPLUS
```

```
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
(30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS
(35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS

L9 ANSWER 22 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
S95548-15-5 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, [1,5-naphthalenedisulfonato(2-)-κO]bis(2-propanamine)-
(9CI) (CA INDEX NAME)

MF C16 H24 Cd N2 O6 S2
CI CCS, COM
SR CA
```

9, 1

# Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
======== C6-C6	=+====================================	+======-  6-6	C10	591.49.57	1

```
ANSWER 23 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     595548-14-4 REGISTRY
Entered STN: 30 Sep 2003
Cadmium, [1,5-naphthalenedisulfonato(2-)-k0]bis(1-propanamine)-,
compd. with 1-propanamine (1:2), dihydrate (9CI) (CA INDEX NAME)
RN
ED
     C16 H24 Cd N2 O6 S2 . 2 C3 H9 N . 2 H2 O
MF
SR
     STN Files:
                  CA, CAPLUS
LÇ
DT.CA CAplus document type: Journal
       Roles from non-patents: PREP (Preparation); PRP (Properties); RACT
       (Reactant or reagent)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                               Ring
Analysis |Sequence | the Rings | Formula | Identifier | Occurrence
                                           | RID | Count
                                  RF
         l ES
                 l SZ
   EΑ
```

C6-C6 | C6-C6 | 6-6 | C10 | 591.49.57 | 1 in CM

CM 1

CRN 595548-13-3

CMF C16 H24 Cd N2 06 S2

CCI CCS

$$0 = \frac{NH_2 - Pr - n}{2 + NH_2 - Pr - n}$$

$$0 = \frac{1}{2 + NH_2} - Pr - n$$

$$0 = \frac{1}{2 + NH_2} - Pr - n$$

$$0 = \frac{1}{2 + NH_2} - Pr - n$$

CM 2 CRN 107-10-8 CMF C3 H9 N

H3C- CH2- CH2- NH2

Experimental Property Tags (ETAG)

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN 139:239001 CA
TI Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
AU Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
CS School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan)
University, Canton, 510275, Peop. Rep. China
SO Journal of Materials Chemistry (2003), 13(7), 1806-1811
CODEN: JMACEP; ISSN: 0959-9428
PB Royal Society of Chemistry

```
DT
        Journal
        English
LA
        78-3 (Inorganic Chemicals and Reactions)
CC
         [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered
AB
        metal sulfonate. It can selectively intercalate ammonia and amines quant.
        without dehydration and form stable adducts, via solid-vapor reaction at
        room temperature The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of
        amine mols. were intercalated by coordinative bonds replacing the
        coordinated water mols., while the extra molar amts. of amines were
        anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed. The intercalation process is
        reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material. cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
ST
         Thermal decomposition
IT
              (of cadmium naphthalenedisulfonate with coordinated/intercalated
              amines)
        Amines, reactions RL: RCT (Reactant); RACT (Reactant or reagent)
IT
              (primary; selective amine coordinative substitution/intercalation
              behavior of cadmium diaqua naphthalenedisulfonate complex)
         Intercalation
IT
              (selective amine coordinative substitution/intercalation behavior of
              cadmium diaqua naphthalenedisulfonate complex)
                                                                                       595548-14-4P
                                                                                                                  595548-16-6P
                                                             595548-12-2P
                                   595548-10-0P
         595548-08-6P
IT
                                                                                       595548-22-4P
                                                              595548-21-3P
                                   595548-20-2P
         RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and thermal decomposition by selective amine coordinative
         595548-18-8P
              substitution/intercalation of cadmium diaqua naphthalenedisulfonate
              complex)
         473251-23-9P
IT
         RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
         (Preparation); RACT (Reactant or reagent)
              (preparation, thermal decomposition and selective amine coordinative
              substitution/intercalation behavior of cadmium diaqua
         naphthalenedisulfonate complex)

81-04-9, 1,5-Naphthalenedisulfonic acid

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
IT
RE.CNT
(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81
(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS
(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS
(4) Cai, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dyer A: An Introduction to Zeolite Molecular Sieves
 (15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
 (16) Eddoudi, M; Acc Chem Res 2001, V34, P319
```

```
(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS (18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS (19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS (20) Kondo M: Angow Chem Tat Ed 1990
(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS
(21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS (24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS (25) Pan, L; Chem Commun 2003, P854 CAPLUS (26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS (27)
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS (33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS (34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS (35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS
        ANSWER 24 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        595548-13-3 REGISTRY
RN
        Entered STN: 30 Sep 2003
ED
        Cadmium, [1,5-naphthalenedisulfonato(2-)-k0]bis(1-propanamine)-
CN
         (9CI) (CA INDEX NAME)
        C16 H24 Cd N2 O6 S2
MF
        CCS, COM
CI
         CA
SR
```

# Ring System Data

Analysis EA	Sequence   ES	the Rings	Ring System   Formula   RF +=======	Identifier   RID	Count
	+======== 		C10	591.49.57	1

```
L9 ANSWER 25 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
RN 595548-12-2 REGISTRY
ED Entered STN: 30 Sep 2003
CN Cadmium, bis(ethanamine)[1,5-naphthalenedisulfonato(2-)-κ0]-, compd.
with ethanamine (1:2), dihydrate (9CI) (CA INDEX NAME)
MF C14 H20 Cd N2 O6 S2 . 2 C2 H7 N . 2 H2 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
```

RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties); RACT (Reactant or reagent)

# Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
c6-c6	c6-c6	6-6	C10	591.49.57	1 in CM  1

CM 1

CRN 595548-11-1

CMF C14 H20 Cd N2 O6 S2

CCI CCS

CM 2

CRN 75-04-7 CMF C2 H7 N

H3C-CH2-NH2

# Experimental Property Tags (ETAG)

, not Entit	OTE
	===== ) CAS
IR Spectra (1	) CAS
X-Ray Diffraction Pattern (1	) CAS

(1) Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

```
139:239001 CA
AN
       Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2]
TI
       Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang
ΑU
       school of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan)
CS
       University, Canton, 510275, Peop. Rep. China
Journal of Materials Chemistry (2003), 13(7), 1806-1811
SO
       CODEN: JMACEP; ISSN: 0959-9428
       Royal Society of Chemistry
PΒ
       Journal
DT
       English
LA
       78-3 (Inorganic Chemicals and Reactions)
[Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered
CC
AB
       metal sulfonate. It can selectively intercalate ammonia and amines quant.
       without dehydration and form stable adducts, via solid-vapor reaction at room temperature. The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M
       amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of
       amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented
       in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid
       phase transformations were also observed The intercalation process is
       reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.
       cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation
ST
       Thermal decomposition
IT
            (of cadmium naphthalenedisulfonate with coordinated/intercalated
            amines)
       Amines, reactions
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
            (primary; selective amine coordinative substitution/intercalation
            behavior of cadmium diaqua naphthalenedisulfonate complex)
       Intercalation
IT
            (selective amine coordinative substitution/intercalation behavior of
            cadmium diaqua naphthalenedisulfonate complex)
                                                                           595548-14-4P
                              595548-10-0P
                                                     595548-12-2P
        595548-08-6P
IT
                                                                           595548-22-4P
                                                     595548-21-3P
        595548-18-8P
                              595548-20-2P
       RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and thermal decomposition by selective amine coordinative
            substitution/intercalation of cadmium diaqua naphthalenedisulfonate
            complex)
        473251-23-9P
IT
       RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
            (preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua
            naphthalenedisulfonate complex)
       81-04-9, 1,5-Naphthalenedisulfonic acid
IT
        RL: RCT (Reactant); RACT (Reactant or reagent)
            (reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
                     THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FO

(1) Cai, J; Chinese J Inorg Chem 2003, V19, P81

(2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS

(3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS

(4) Cai, J; Unpublished results

(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS

(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS

(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
```

```
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dver A: An Introduction to Zeolite Molecular Sieves
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988
(16) Eddoudi, M; Acc Chem Res 2001, V34, P319

(17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS

(18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS

(19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS

(20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS

(21) Li, H; Nature 1999, V402, P276 CAPLUS

(22) Makinen, S: Chem Fur J 2001, V4, P5176
(21) L1, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Commun 2003, P854 CAPLUS
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS
(28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS
(29) Querler, L; C R Acad Sci Ser C 1972, V275, P321
(30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS
(31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
 (31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS
 (32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
 (33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS (34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS (35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS
              ANSWER 26 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
 L9
               595548-11-1 REGISTRY
 RN
               Entered STN: 30 Sep 2003
 ED
              Cadmium, bis(ethanamine)[1,5-naphthalenedisulfonato(2-)-κ0]- (9CI)
 CN
               (CA INDEX NAME)
              C14 H20 Cd N2 O6 S2
 MF
 CI
               CCS, COM
               CA
 SR
 Ring System Data
```

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
= <b>======</b> - C6-C6	+=======   c6-c6	6-6	C10	591.49.57	1

# Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
c6-c6	C6-C6	6-6	C10	591.49.57.	1 in CM  1

CRN 595548-09-7 CMF C12 H16 Cd N2 O6 S2

CCI CCS

CRN 74-89-5 CMF C H5 N

H<sub>3</sub>C-NH<sub>2</sub>

Experimental Property Tags (ETAG)

	NO	
IR Spectra X-Ray Diffraction Pattern		_

Cai, Jiwen; Journal of Materials Chemistry 2003 V13(7) P1806-1811 (1)**CAPLUS** 

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

139:239001 CA AN Selective amine intercalation behavior of [Cd(1,5-nds)(H2O)2] TI

Cai, Jiwen; Zhou, Jin-Sen; Lin, Mu-Liang ΑU School of Chemistry and Chemical Engineering, Sun Yat-Sen (Zhongshan) CS

University, Canton, 510275, Peop. Rep. China Journal of Materials Chemistry (2003), 13(7), 1806-1811 SO CODEN: JMACEP; ISSN: 0959-9428

Royal Society of Chemistry PB

Journal DT English LA

CC

English 78-3 (Inorganic Chemicals and Reactions) [Cd(1,5-nds)(H2O)2] (1,5-nds = 1,5-naphthalenedisulfonate) is a layered metal sulfonate. It can selectively intercalate ammonia and amines quant. without dehydration and form stable adducts, via solid-vapor reaction at room temperature. The resulting adducts were characterized by elemental analyses, IR, TGA-IR and PXRD. The title compound can absorb up to 4 M amts. of C2H5NH2 and PrNH2. TGA-IR analyses show that amines were intercalated by interactions of different nature. Of these, 2 M amts. of AB amine mols. were intercalated by coordinative bonds replacing the coordinated water mols., while the extra molar amts. of amines were anchored by weak but steady intermol. interactions, which is unprecedented in metal phosphate or sulfonate analogs. Guest-driven solid-to-solid phase transformations were also observed The intercalation process is reversible, selective and preferential, indicating that the title compound could be designed as an amine-sensitive material.

cadmium aqua naphthalenedisulfonate prepn amine substitution intercalation ST

Thermal decomposition IT

(of cadmium naphthalenedisulfonate with coordinated/intercalated amines)

IT

RL: RCT (Reactant); RACT (Reactant or reagent) (primary; selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

Intercalation IT (selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

595548-12-2P ... 595548-14-4P 595548-16-6P 595548-10-0P 595548-08-6P IT 595548-22-4P 595548-21-3P 595548-20-2P 595548-18-8P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and thermal decomposition by selective amine coordinative substitution/intercalation of cadmium diaqua naphthalenedisulfonate complex)

473251-23-9P IT RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, thermal decomposition and selective amine coordinative substitution/intercalation behavior of cadmium diaqua naphthalenedisulfonate complex)

81-04-9, 1,5-Naphthalenedisulfonic acid

RL: RCT (Reactant); RACT (Reactant or reagent)

IT

```
(reactant for preparation of cadmium diaqua naphthalenedisulfonate complex)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD (1) Cai, J; Chinese J Inorg Chem 2003, V19, P81 (2) Cai, J; J Chem Soc, Dalton Trans 2001, P1137 CAPLUS (3) Cai, J; J Chem Soc, Dalton Trans 2001, P2370 CAPLUS (4) Cai, J; Unpublished results (5) Cao, G: Chem Mater 1003, V5, P1000, CAPLUS
(4) Ca1, J; Unpublished results
(5) Cao, G; Chem Mater 1993, V5, P1000 CAPLUS
(6) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(7) Chen, C; Inorg Chem 2002, V41, P4967 CAPLUS
(8) Chen, C; J Chem Crystallogr 2001, V3, P271
(9) Chui, S; Science 1999, V283, P1148 CAPLUS
(10) Clearfield, A; J Chem Soc, Dalton Trans 2002, P2973
(11) Clearfield, A: Prog. Thorg Chem 1998, V47, P371 CAPLUS
(11) Clearfield, A; Prog Inorg Chem 1998, V47, P371 CAPLUS
(12) Cote, A; Chem Commun 2001, P251 CAPLUS
(13) Cote, A; Inorg Chem 2002, V41, P287 CAPLUS
(14) Cussen, E; J Am Chem Soc 2002, V124, P9574 CAPLUS
(15) Dyer, A; An Introduction to Zeolite Molecular Sieves 1988 (16) Eddoudi, M; Acc Chem Res 2001, V34, P319 (17) Edgar, M; Chem Eur J 2001, V7, P5168 CAPLUS (18) Fredoueil, F; Inorg Chem 1999, V38, P1831 CAPLUS (19) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS (20) Kondo, M; Angew Chem, Int Ed 1999, V38, P140 CAPLUS (21) Li Li Nature 1999, V402 P276 CAPLUS
 (21) Li, H; Nature 1999, V402, P276 CAPLUS
(22) Makinen, S; Chem Eur J 2001, V4, P5176
(23) Min, K; J Am Chem Soc 2000, V122, P6834 CAPLUS
(24) Pan, L; Angew Chem, Int Ed 2003, V42, P542 CAPLUS
(25) Pan, L; Chem Comun 2003, P854 CAPLUS
(26) Pan, L; J Am Chem Soc 2003, V125, P3062 CAPLUS
(27) Papaefstathiou, G; Angew Chem, Int Ed 2002, V41, P2070 CAPLUS (28) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS (29) Querler, L; C R Acad Sci Ser C 1972, V275, P321 (30) Shimizu, G; Chem Mater 1998, V10, P3282 CAPLUS (31) Yaghi, O; Acc Chem Res 1998, V31, P474 CAPLUS (32) Zaworotko M: Nature 1000 V402 P242 CAPLUS
 (32) Zaworotko, M; Nature 1999, V402, P242 CAPLUS
(33) Zhang, X; Eur J Inorg Chem 2003, P138 CAPLUS
(34) Zhang, Y; Chem Mater 1993, V5, P495 CAPLUS (35) Zhang, Y; Inorg Chem 1992, V31, P2821 CAPLUS
           ANSWER 28 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
           595548-09-7 REGISTRY
RN
           Entered STN: 30 Sep 2003
ED
           Cadmium, bis(methanamine)[1,5-naphthalenedisulfonato(2-)-\kappa0]- (9CI)
CN
           (CA INDEX NAME)
           C12 H16 Cd N2 O6 S2
MF
CI
           CCS, COM
SR
           CA
Ring System Data
                                                                                                Ring
Elemental|Elemental| Size of |Ring System|
                                                                                         |Identifier|Occurrence
Analysis |Sequence | the Rings | Formula
                                                                                                           | Count
                                                                                         RID
                                         SZ
                                                                        RF
       EΑ
                            ES
                                                             =+=======
                                                                                      =+===================
|591.49.57 |1
                                                               |C10
```

C6-C6

|C6-C6

6-6

```
ANSWER 29 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
      550305-04-9 REGISTRY
RN
      Entered STN: 18 Jul 2003
ED
      Silver(2+), bis(1-propanamine)[\mu-[1,1'-thiobis[ethane]]]di-, dinitrite (9CI) (CA INDEX NAME)
CN
      C10 H28 Ag2 N2 S . 2 N O2
MF
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAPlus document type: Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
SR
      CM
      CRN 550305-03-8
      CMF C10 H28 Ag2 N2 S
      CCI CCS
    Ag + NH2-Pr-n
    A'g^{+}NH_2-Pr-n
```

CM 2 CRN 14797-65-0 CMF N 02

o== N- o-

Experimental Property Tags (ETAG)

(1) Jung, Won Cheol; EP 1323721 A2 2003 CAPLUS

See HELP PROPERTIES for information about property data sources in REGISTRY. 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE) REFERENCE 1 139:77881 CA AN Metal thioether complexes as organic metal precursors for use in forming metal-containing patterned films
Jung, Won Cheol; Chang, Seok; Hwang, Soon Taik; Byun, Young Hun
Samsung Electronics Co., Ltd., S. Korea TI IN PA Eur. Pat. Appl., 8 pp. SO CODEN: EPXXDW Patent DT English LA ICM C07F001-00 IC ICS C07F003-00; C07F015-00; C07F015-06; C07F015-04; C23C016-00 78-7 (Inorganic Chemicals and Reactions) CC Section cross-reference(s): 74 FAN.CNT 1 APPLICATION NO. DATE KIND DATE PATENT NO. 20021111 EP 2002-257784 20030702 EP 1323721 A2 ΡI 20031008 Α3 EP 1323721 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK 057133 A 20030704 KR 2001-87510 20011228 124457 A1 20030703 US 2002-282031 20021029 KR 2003057133 us 2003124457 20051115 В2 us 6965045 JP 2002-373621 20021225 20031010 **A2** JP 2003286579 20011228 PRAI KR 2001-87510 Disclosed are organic metal precursors comprising one or more thioether ligands bonded to one or more metal atoms (metal = Ag, Au, Co, Cu, Pd, Ni, Pt, Zn, Cd), wherein the organic ligand is rapidly dissociated from the metal atom upon exposure to light and degraded leaving a metal or a metal oxide. Thus, reaction of AgNo2 and Et2S in heated MeCN afforded Thus, reaction of AgNO2 and Et2s in heated MeCN afforded [(Et2s)Ag+](NO2-). Reaction of the latter with PrNH2 in MeCN afforded [(PrNH2)Ag]2SEt2. Using the organic metal precursors of the present invention, e.g., [(PrNH2)Ag]2SEt2, an electroconductive, metal-containing patterned film can be easily deposited on a substrate at room temperature under atmospheric pressure without using photosensitive resins. transition metal thioether complex prepn photodegrdn; patterned silver film prepn photodegrdn thioether complex precursor; silver thioether complex prepn photodegrdn patterned film precursor ST Films IT (elec. conductive, patterned; preparation of metal thioether complexes and their photodegrdn. to form metal-containing patterned films without use of photosensitive resins) Electric conductors IT (films, patterned; preparation of metal thioether complexes and their photodegrdn. to form metal-containing patterned films without use of photosensitive resins) Transition metal complexes IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (thioether; preparation of metal thioether complexes and their photodegrdn. to form metal-containing patterned films without use of photosensitive resins)

(complexation with silver thioether complex to give precursor of

107-10-8, Propylamine, reactions RL: RCT (Reactant); RACT (Reactant or reagent)

IT

```
silver-containing patterned films)
     60-29-7, Diethyl ether, reactions 110-01-0, Tetrahydrothiophene 7761-88-8, Silver nitrate, reactions 7783-99-5, Silver nitrite
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (complexation with thioethers to give precursors of silver-containing
        patterned films)
                     550305-01-6P
                                     550305-02-7P
     550304-99-9P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation as precursor for use in forming metal-containing patterned
film)
     550305-04-9P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation as precursor for use in forming metal-containing patterned
film via
        photodegrdn. without use of photosensitive resins)
     ANSWER 30 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN.
L9
     550305-03-8 REGISTRY
RN
                   18 Jul 2003
     Entered STN:
     Silver(2+), bis(1-propanamine)[\mu-[1,1'-thiobis[ethane]]]di- (9CI) (CA
ED
CN
     INDEX NAME)
     C10 H28 Ag2 N2 S
MF
     CCS, COM
CI
     CA
SR
   Ag<sup>+</sup> NH2-Pr-n
Et-S-Et
   Ag + NH2-Pr-n
     ANSWER 31 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     284476-55-7 REGISTRY
RN
     Entered STN: 09 Aug 2000
ED
     Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-23)- (9CI) (CA
CN
     INDEX NAME)
     C2 H17 CO N 04 S
MF
     CCS
CI
SR
     CA
     STN Files:
                   CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)
      SH-Me
      NH2-Me
```

# 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

```
133:125569 CA
ΑN
              Ab Initio calculations of [CoY6-nXn]2+ complexes Rulisek, Lubomir; Havlas, Zdenek
TI
             Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic, Prague, 166 10, Czech Rep. Journal of Chemical Physics (2000), 112(1), 149-157
ΑU
CS
SO
              CODEN: JCPSA6; ISSN: 0021-9606
American Institute of Physics
PB
              Journal
DT
              English
LA
              65-5 (General Physical Chemistry)
            Section cross-reference(s): 6, 68, 78
The CASSCF and multi-reference second order perturbation theory (CASPT2)
calcns. of [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+ and
[Co(H2O)4X2]2+ complexes (X = CH3OH, CH3SH, CH3NH2) are reported. The
potential energy surfaces of 10 lowest quartet states of [Co(H2O)5X]2+
complexes near the equilibrium geometry are calculated and splitting of
triple-degenerate 4T1g(F), 4T2g(F), and 4T1g(P) electronic states of
[Co(H2O)6]2+ complex induced by the substitution of one or two water
ligands is characterized and quantified. The energy differences between
originally degenerate states are almost invariant to the changes of
metal-ligand distances, and despite their proximity, the crossing does not
occur. The coeffs. of the leading configuration of multi-reference wave
functions of [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes are shown to
approach unity and the usage of single-reference methods is justified. As a
consequence, interaction energies of the studied functional groups with
CO2+ are computed also at the HF, DFT and MP2 levels. They are compared
to CASSCF calcns. and to the equivalent calcns. done for Zn2+ and Ni2+ ions.
The computational methodol. for the accurate calcns. of various cobalt
(II) ionic complexes is described and the implications for the theor.
CC
              Section cross-reference(s): 6, 68, 78
AB
               (II) ionic complexes is described and the implications for the theor.
               investigation of interactions of chemical and biol. important functional
               groups with Co2+ are discussed.
              cobalt mixed ligand complex CASSCF CASPT2 HF MP2 DFT; potential surface cobalt mixed ligand complex; quartet state PES cobalt mixed ligand complex; degenerate state cobalt mixed ligand complex PES; fluoride cobalt mixed ligand complex PES; fluoride cobalt
 ST
              complex electronic structure geometry; water mixed ligand complex cobalt electronic structure geometry; ammonia mixed ligand complex cobalt electronic structure geometry; methylamine mixed ligand complex cobalt electronic structure geometry; methylamine mixed ligand complex cobalt electronic structure geometry; methanol mixed ligand complex cobalt electronic structure geometry; methanethiol mixed ligand complex cobalt electronic structure geometry
               electronic structure geometry
Bond length
 IT
               Electronic excitation
               Energy level splitting Ground state
               Jahn-Teller effect
               Molecular structure
                Potential energy surface
                        (ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+,
                        [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH,
                        CH3NH2))
               Electronic state
 IT
                        (quartet; ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+,
                        [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3SH)
                        CH3NH2))
  IT
               Energy
```

```
(substitution-reaction; ab initio calcns. of cobalt complexes [CoF6]4-,
                 [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH, CH3NH2))
15276-47-8, Hexaaquacobalt(2+)
15365-75-0, Hexaamminecobalt(2+)
                                                            29868-74-4, Hexafluorocobaltate(4-) 60119-04-2 60119-05-3
IT
                 29858-93-3
                                                                                                          223243-89-8 223243-91-2 282542-77-2
                                                            125823-87-2
                 79231-71-3
                                                                                                                                                                                                           284476-55-7
                                                                                                                                                           282550-54-3
                                                                                                              282549-07-9
                                                              282547-97-1
                 282547-96-0
                                                               284476-58-0
                 284476-56-8
                 RL: PRP (Properties)
                            (ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+,
                            [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH,
                            CH3NH2))
                                              THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD
                           64
 (1) Akesson, R; J Am Chem Soc 1994, V116, P8691

(2) Akesson, R; J Am Chem Soc 1994, V116, P8705

(3) Akesson, R; J Phys Chem 1992, V96, P10773

(4) Akesson, R; J Phys Chem 1992, V96, P150

(5) Akesson, R; J Phys Chem 1993, V97, P3765 CAPLUS

(6) Allen, G; J Chem Soc A 1970, P2668, CAPLUS

(7) Rarone, V: Int. J Quantum Chem 1997, V61, P443 C.
 RE.CNT
 (7) Barone, V; Int J Quantum Chem 1997, V61, P443 CAPLUS
(8) Becke, A; J Chem Phys 1993, V98, P5648 CAPLUS
(9) Becke, A; Phys Rev A 1988, V38, P3098 CAPLUS
(10) Bertini, I; Handbook of Metal-Ligand Interactions in Biological Fluids
1995, V1, P81 CAPLUS
(11) Bathor H: App Phys (Leipzig) 1972, V2, P122
  (11) Bethe, H; Ann Phys (Leipzig) 1972, V3, P133
(12) Blyholder, G; Theor Chim Acta 1982, V60, P429 CAPLUS
(13) Broclawik, E; J Mol Catal 1993, V82, P117 CAPLUS
  (14) Brunschwig, B; Faraday Discuss Chem Soc 1982, V74, P113
  (15) Clark, T; J Comput Chem 1983, V4, P294 CAPLUS (16) Cory, M; Chem Rev 1991, V91, P813 CAPLUS
(15) Clark, 1; J Comput Cnem 1983, V4, P294 CAPLUS
(16) Cory, M; Chem Rev 1991, V91, P813 CAPLUS
(17) Cotton, F; Advanced Inorganic Chemistry, 4th ed 1980
(18) Cotton, F; J Am Chem Soc 1997, V119, P7514 CAPLUS
(19) Dalgaard, E; J Chem Phys 1978, V69, P3833 CAPLUS
(20) De Kerpel, J; J Phys Chem B 1999, V103, P8375 CAPLUS
(21) Delley, B; J Chem Phys 1994, V100, P5785 CAPLUS
(22) Edwards, W; J Am Chem Soc 1986, V108, P2196 CAPLUS
(23) Edwards, W; J Phys Chem 1988, V92, P6188 CAPLUS
(24) Filatov, M; Theor Chim Acta 1987, V72, P211 CAPLUS
(25) Fournier, R; J Chem Phys 1995, V102, P5396 CAPLUS
(26) Frausto da Silva, J; The Biological Chemistry of the Elements 1993
(27) Frisch, M; GAUSSIAN 98. Revision A.6 1998
(28) Frisch, M; J Chem Phys 1984, V80, P3265 CAPLUS
(39) Garmer, D; J Am Chem Soc 1992, V114, P6487 CAPLUS
(30) Geselowitz, D; Inorg Chim Acta 1989, V163, P79 CAPLUS
(31) Gilson, H; J Phys Chem A 1998, V102, P6525 CAPLUS
(32) Glukhovtsev, M; J Phys Chem A 1997, V101, P316 CAPLUS
(33) Glusker, J; Adv Protein Chem 1991, V42, P1 CAPLUS
(34) Hay, P; J Chem Phys 1977, V66, P4377 CAPLUS
(35) Hegarty, D; Mol Phys 1979, V38, P1795 CAPLUS
(36) Holmes, O; J Chem Phys 1957, V26, P1686 CAPLUS
(37) Jorgensen, C; Acta Chem Scand 1964, V18, P1495
(38) Kime, N; Acta Crystallogr, Sect B: Struct Crystallogr Cryst Chem 1969, V25, P168 CAPLUS
                V25, P168 CAPLUS
  (39) Klopper, W; Chem Phys Lett 1996, V262, P546 CAPLUS (40) Kotzian, M; J Am Chem Soc 1989, V111, P7687 CAPLUS (41) Krishnan, R; J Chem Phys 1980, V72, P650 CAPLUS (42) Lee, C; Phys Rev B 1980, V37, P785 (43) Marcus, Y; Chem Rev 1988, V88, P1475 CAPLUS (44) McDouall, J; Chem Phys Lett 1988, V148, P183 CAPLUS (45) McLean, A; J Chem Phys 1980, V72, P5639 CAPLUS (46) Newton, M; J Phys Chem 1991, V95, P30 CAPLUS
```

```
(47) Papai, I; J Chem Phys 1995, V103, P1860 CAPLUS
(48) Raghavachari, K; J Chem Phys 1989, V91, P1062
(49) Rodriguez-Santiago, L; Can J Chem 1996, V105, P9966 CAPLUS
(50) Rosi, M; J Chem Phys 1990, V92, P1876 CAPLUS
(50) Rosi, M; J Chem Phys 1990, V92, P1876 CAPLUS (51) Rulisek, L; J Inorg Biochem 1998, V71, P115 CAPLUS (52) Rulisek, L; J Phys Chem A 1999, V103, P1634 CAPLUS (53) Schmidt, M; J Comput Chem 1993, V14, P1347 CAPLUS (54) Siegbahn, P; J Chem Phys 1981, V74, P2384 (55) Soudackov, A; Theor Chim Acta 1992, V83, P389 (56) Taketsugu, T; J Chem Phys 1997, V106, P8504 CAPLUS (57) Thomas, J; J Phys Chem A 1997, V101, P8530 CAPLUS (58) Veillard, A; Chem Rev 1991, V91, P743 CAPLUS (59) Vosko, S; Can J Phys 1980, V58, P1200 CAPLUS
(59) Vosko, S; Can J Phys 1980, V58, P1200 CAPLUS (60) Waizumi, K; Chem Lett 1992, P1489 CAPLUS
(61) Watchers, A; J Chem Phys 1970, V52, P1033
(62) Zerner, M; J Am Chem Soc 1980, V102, P589 CAPLUS (63) Ziegler, T; Can J Chem 1994, V72, P783 CAPLUS (64) Ziegler, T; Chem Rev 1991, V91, P651 CAPLUS
          ANSWER 32 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
          282547-96-0 REGISTRY
Entered STN: 02 Aug 2000
RN
ED
          Cobalt(2+), tetraaqua(methanamine)(methanethiol)-, (OC-6-32)- (9CI) (CA
          INDEX NAME)
          C2 H17 CO N O4 S
MF
          CCS
CI
SR
          CA
                                    CA, CAPLUS
          STN Files:
LC
DT.CA CAplus document type:
                                                           Journal
RL.NP Roles from non-patents: PRP (Properties)
             SH-Me
                    OH<sub>2</sub>
H20
            NH2-Me
                               1 REFERENCES IN FILE CA (1907 TO DATE)
                               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
           133:125569 CA
AN
          Ab Initio calculations of [CoY6-nXn]2+ complexes Rulisek, Lubomir; Havlas, Zdenek
 TI
ΑU
          Institute of Organic Chemistry and Biochemistry, Academy of Science of the Czech Republic, Prague, 166 10, Czech Rep.
Journal of Chemical Physics (2000), 112(1), 149-157
CODEN: JCPSA6; ISSN: 0021-9606
CS
SO
           American Institute of Physics
 PB
DT
           Journal
LA
           English
           65-5 (General Physical Chemistry)
CC
           Section cross-reference(s): 6, 68, 78
```

```
The CASSCF and multi-reference second order perturbation theory (CASPT2) calcns. of [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes (X = CH3OH, CH3SH, CH3NH2) are reported. The potential energy surfaces of 10 lowest quartet states of [Co(H2O)5X]2+
AΒ
          complexes near the equilibrium geometry are calculated and splitting of triple-degenerate 4Tlg(F), 4T2g(F), and 4Tlg(P) electronic states of [Co(H2O)6]2+ complex induced by the substitution of one or two water ligands is characterized and quantified. The energy differences between
          originally degenerate states are almost invariant to the changes of
          metal-ligand distances, and despite their proximity, the crossing does not occur. The coeffs. of the leading configuration of multi-reference wave
         occur. Ine coeffs. of the leading configuration of multi-reference wave functions of [Co(H2O)5X]2+ and [Co(H2O)4X2]2+ complexes are shown to approach unity and the usage of single-reference methods is justified. As a consequence, interaction energies of the studied functional groups with Co2+ are computed also at the HF, DFT and MP2 levels. They are compared to CASSCF calcns. and to the equivalent calcns. done for Zn2+ and Ni2+ ions. The computational methodol. for the accurate calcns. of various cobalt (II) ionic complexes is described and the implications for the theor. investigation of interactions of chemical and biol important functional
           investigation of interactions of chemical and biol. important functional
          groups with Co2+ are discussed.
cobalt mixed ligand complex CASSCF CASPT2 HF MP2 DFT; potential surface cobalt mixed ligand complex; quartet state PES cobalt mixed ligand
ST
           complex; degenerate state cobalt mixed ligand complex PES; fluoride cobalt
          complex electronic structure geometry; water mixed ligand complex cobalt electronic structure geometry; ammonia mixed ligand complex cobalt electronic structure geometry; methylamine mixed ligand complex cobalt electronic structure geometry; methanol mixed ligand complex cobalt electronic structure geometry; methanol mixed ligand complex cobalt electronic structure geometry; methanethiol mixed ligand complex cobalt electronic structure geometry; methanethiol mixed ligand complex cobalt
           electronic structure geometry
           Bond length
IT
           Electronic excitation
           Energy level splitting
Ground state
           Jahn-Teller effect
           Molecular structure
           Potential energy surface
                  (ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH,
                  CH3NH2))
IT
           Electronic state
                  (quartet; ab initio_calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+,
                  [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH,
                  CH3NH2)
IT
                  (substitution-reaction; ab initio calcns. of cobalt complexes [CoF6]4-,
                  [Co(H2O)6]2+, [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X =
                                      Hexaaquacobalt(2+) 15365-75-0, Hexaamminecobalt(2+) 29868-74-4, Hexafluorocobaltate(4-) 60119-04-2 60119-05-3 125823-87-2 223243-89-8 223243-91-2 282542 77 3
                  CH30H, CH3SH, CH3NH2))
           15276-47-8, Hexaaquacobalt(2+)
IT
           29858-93-3
           79231-71-3
                                                                                                     282550-54-3
                                                                                                                                   284476-55-7
                                                                       282549-07-9
           282547-96-0
                                         282547-97-1
                                         284476-58-0
           284476-56-8
           RL: PRP (Properties)
                  (ab initio calcns. of cobalt complexes [CoF6]4-, [Co(H2O)6]2+,
                  [Co(NH3)6]2+, [Co(H2O)5X]2+, and [Co(H2O)4X2]2+ (X = CH3OH, CH3SH,
                  CH3NH2))
                              THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Akesson, R; J Am Chem Soc 1994, V116, P8691
(2) Akesson, R; J Am Chem Soc 1994, V116, P8705
(3) Akesson, R; J Phys Chem 1992, V96, P10773
(4) Akesson, R; J Phys Chem 1992, V96, P150
```

```
(5) Akesson, R; J Phys Chem 1993, V97, P3765 CAPLUS
 (6) Allen, G; J Chem Soc A 1970, P2668 CAPLUS
 (7) Barone, V; Int J Quantum Chem 1997, V61, P443 CAPLUS
(8) Becke, A; J Chem Phys 1993, V98, P5648 CAPLUS (9) Becke, A; Phys Rev A 1988, V38, P3098 CAPLUS
(10) Bertini, I; Handbook of Metal-Ligand Interactions in Biological Fluids
(11) Bethe, H; Ann Phys (Leipzig) 1972, V3, P133
(12) Blyholder, G; Theor Chim Acta 1982, V60, P429 CAPLUS
(13) Broclawik, E; J Mol Catal 1993, V82, P117 CAPLUS
(14) Brunschwig, B; Faraday Discuss Chem Soc 1982, V74, P113
(15) Clark, T; J Comput Chem 1983, V4, P294 CAPLUS
(16) Cory, M; Chem Rev 1991, V91, P813 CAPLUS
(17) Cotton, F; Advanced Thorganic Chemistry, 4th, ed 1980
               1995, V1, P81 CAPLUS
(17) Cotton, F; Advanced Inorganic Chemistry, 4th ed 1980 (18) Cotton, F; J Am Chem Soc 1997, V119, P7514 CAPLUS (19) Dalgaard, E; J Chem Phys 1978, V69, P3833 CAPLUS
(20) De Kerpel, J; J Phys Chem B 1999, V103, P8375 CAPLUS (21) Delley, B; J Chem Phys 1994, V100, P5785 CAPLUS
(21) Delley, B; J Chem Phys 1994, V100, P5/85 CAPLUS
(22) Edwards, W; J Am Chem Soc 1986, V108, P2196 CAPLUS
(23) Edwards, W; J Phys Chem 1988, V92, P6188 CAPLUS
(24) Filatov, M; Theor Chim Acta 1987, V72, P211 CAPLUS
(25) Fournier, R; J Chem Phys 1995, V102, P5396 CAPLUS
(26) Frausto da Silva, J; The Biological Chemistry of the Elements 1993
(27) Frisch, M; GAUSSIAN 98. Revision A.6 1998
(28) Frisch, M; J Chem Phys 1984, V80, P3265 CAPLUS
(29) Garmer, D; J Am Chem Soc 1992, V114, P6487 CAPLUS
(28) Frisch, M; J Chem Phys 1984, V80, P3265 CAPLUS
(29) Garmer, D; J Am Chem Soc 1992, V114, P6487 CAPLUS
(30) Geselowitz, D; Inorg Chim Acta 1989, V163, P79 CAPLUS
(31) Gilson, H; J Phys Chem A 1998, V102, P6525 CAPLUS
(32) Glukhovtsev, M; J Phys Chem A 1997, V101, P316 CAPLUS
(33) Glusker, J; Adv Protein Chem 1991, V42, P1 CAPLUS
(34) Hay, P; J Chem Phys 1977, V66, P4377 CAPLUS
(35) Hegarty, D; Mol Phys 1979, V38, P1795 CAPLUS
(36) Holmes, O; J Chem Phys 1957, V26, P1686 CAPLUS
(37) Jorgensen, C; Acta Chem Scand 1964, V18, P1495
(38) Kime, N; Acta Crystallogr, Sect B: Struct Crystallogr Cryst Chem 1969, V25, P168 CAPLUS
V25, P168 CAPLUS

(39) Klopper, W; Chem Phys Lett 1996, V262, P546 CAPLUS

(40) Kotzian, M; J Am Chem Soc 1989, V111, P7687 CAPLUS

(41) Krishnan, R; J Chem Phys 1980, V72, P650 CAPLUS

(42) Lee, C; Phys Rev B 1980, V37, P785

(43) Marcus, Y; Chem Rev 1988, V88, P1475 CAPLUS

(44) McDouall, J; Chem Phys Lett 1988, V148, P183 CAPLUS

(45) McLean, A; J Chem Phys 1980, V72, P5639 CAPLUS

(46) Newton, M; J Phys Chem 1991, V95, P30 CAPLUS

(47) Papai, I; J Chem Phys 1995, V103, P1860 CAPLUS

(48) Raghavachari, K; J Chem Phys 1989, V91, P1062

(49) Rodriguez-Santiago, L; Can J Chem 1996, V105, P9966 CAPLUS

(50) Rosi, M; J Chem Phys 1990, V92, P1876 CAPLUS

(51) Rulisek, L; J Inorg Biochem 1998, V71, P115 CAPLUS
               V25, P168 CAPLUS
  (51) Rulisek, L; J Inorg Biochem 1998, V71, P115 CAPLUS
 (52) Rulisek, L; J Phys Chem A 1999, V103, P1634 CAPLUS (53) Schmidt, M; J Comput Chem 1993, V14, P1347 CAPLUS (54) Siegbahn, P; J Chem Phys 1981, V74, P2384 (55) Soudackov, A; Theor Chim Acta 1992, V83, P389 (56) Taketsugu T; J Chem Phys 1907, V106, P8504 CAPLUS
  (56) Taketsugu, T; J Chem Phys 1997, V106, P8504 CAPLUS (57) Thomas, J; J Phys Chem A 1997, V101, P8530 CAPLUS
 (58) Veillard, A; Chem Rev 1991, V91, P743 CAPLUS (59) Vosko, S; Can J Phys 1980, V58, P1200 CAPLUS (60) Waizumi, K; Chem Lett 1992, P1489 CAPLUS
  (61) Watchers, A; J Chem Phys 1970, V52, P1033
(62) Zerner, M; J Am Chem Soc 1980, V102, P589 CAPLUS
  (63) Ziegler, T; Can J Chem 1994, V72, P783 CAPLUS
```

```
Page 130
```

```
(64) Ziegler, T; Chem Rev 1991, V91, P651 CAPLUS
      ANSWER 33 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
      279674-00-9 REGISTRY
RN
      Entered STN: 24 Jul 2000
ED
     Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-\kappa0]-, (OC-6-23)-, perchlorate (9CI) (CA INDEX NAME)
CN
      C H17 CO N5 04 S . Cl 04
MF
      CA
SR
LC STN Files: CA, CAPLUS
DT.CA CAPlus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)
            1
      CM
           210574-34-8
      CRN
           C H17 CO N5 O4 S
      CMF
      CCI CCS
       NH2-Me
            NH3
H3N
            NH<sub>3</sub>
H<sub>3</sub>N′
       0-S03-
            2
      CM
            14797-73-0
      CRN
            cl 04
      CMF
                  1 REFERENCES IN FILE CA (1907 TO DATE)
                  1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      133:79995 CA
AN
      Inductive effect of methyl groups on acidopentaaminecobalt(III) complexes
TI
      Benzo, Fabian; Beyer, Lothar; Bozoglian, Fernando; Hallmeier, Karl-Heinz;
ΑU
      Sienra, Beatriz
      Universidad de la Republica, Catedra de Quimica Inorganica, Montevideo,
CS
      Urug.
      Polyhedron (2000), 19(8), 971-974
CODEN: PLYHDE; ISSN: 0277-5387
SO
      Elsevier Science Ltd.
PB
DT
      Journal
```

```
LA
        67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
         Section cross-reference(s): 78
        Electron spectroscopy for chemical anal. (ESCA) was performed for [Co(NH3)5Cl](Cl04)2, trans-[Co(NH3)4(NH2CH3)Cl]-(Cl04) 2, [Co(NH2CH3)5Cl](Cl04)2 and trans-[Co(NH3)4(NH2CH3)(0SO3)](Cl 04) complexes. Comparison of the results for the complexes
AB
         [Co(NH3)5Cl](Cl04)2 and trans-[Co(NH3)4(NH2CH3)Cl](Cl04)2 shows clearly the electronic influence (+I effect) of the methylamine group on the
         cobalt and through this on the chlorine atom in trans position.
         Comparison of [Co(NH2CH3)5Cl](ClO4)2 with trans-
         [Co(NH3)4(NH2CH3)Cl](ClO4)2 shows that methylation of the four cis-NH3
         ligands does not produce a proportional decrease in the binding energy of
         the cobalt atom, while the electron d. of the chloro ligand is not affected. For the complex trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) the +I effect is almost completely compensated by the presence of the sulfato
         group in trans position. Acid dissociation consts. are also reported for [Co(NH3)5(OH2)]3+ and trans-[Co(NH3)4(NH2CH3)(OH2)]3 + ions. The implications of these results for the mechanism of the acid and base
         hydrolysis reactions of acidopentaaminecobalt(III) complexes are discussed. The preparation of the trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4)
         complex through the trans-[Co(NH3)4(NH2CH3)(SO3)]+ precursor is also
         described.
         inductive effect methyl group acido amine cobalt complex
ST
         Hydrolysis
IT
               (acid, mechanism; inductive effect of Me groups on
               acidopentaaminecobalt(III) complexes)
         Dissociation constant
IT
               (acid; inductive effect of Me groups on acidopentaaminecobalt(III)
               complexes)
         Hydrolysis
IT
               (base, mechanism; inductive effect of Me groups on
               acidopentaaminecobalt(III) complexes)
         Inductive effect
IT
         Methyl group
               (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
                                                         91321-36-7
                                                                                 279674-00-9
                                 15392-60-6
         15156-18-0
IT
         RL: PRP (Properties)
               (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
                                                         134066-32-3
                                 68250-09-9
IT
         14403-82-8
          RL: RCT (Reactant); RACT (Reactant or reagent)
               (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Balt, S; J Chem Soc, Dalton Trans 1983, P2415 CAPLUS (2) Balt, S; Transition Met Chem 1984, V9, P224 CAPLUS (3) Benzo, F; J Chem Crystallogr 1998, V28, P69 CAPLUS (4) Benzo, F; Polyhedron 1915, V15, P1996 (5) Benzo, F; to be published in Inorg React Mechanims
RE.CNT
 (6) Benzo, F; to be published in J Chem Soc, Dalton Trans
(b) Benzo, F; to be published in J Chem Soc, Dalton Trans (7) Brasch, N; Inorg Chem 1989, V28, P4567 CAPLUS (8) Buckingham, D; Inorg Chem 1970, V9, P1790 CAPLUS (9) Buckingham, D; Inorg Chem 1970, V9, P655 CAPLUS (10) Buckingham, D; J Am Chem Soc 1967, V89, P5129 CAPLUS (11) Curtis, N; Inorg Chem 1986, V25, P1033 CAPLUS (12) Curtis, N; Inorg Chem 1986, V25, P484 CAPLUS (13) Curtis, N; Inorg Chem 1989, V28, P329 CAPLUS (14) Dixon, N; Inorg Chem 1982, V21, P688 CAPLUS (15) Foxman, B; Inorg Chem 1932, V17, P1978 (16) Gonzalez, G: Inorg Chem 1994, V33, P2330 CAPLUS
 (16) Gonzalez, G; Inorg Chem 1994, V33, P2330 CAPLUS (17) Jackson, W; Inorg Chem 1984, V23, P2473 CAPLUS (18) Jordan, R; Inorg Chem 1996, V35, P3725 CAPLUS
```

```
(19) Kitamura, Y; Inorg Chem 1989, V28, P333 CAPLUS
 (20) Lawrence, G; Inorg Chem 1984, V23, P3922
(20) Lawrence, G; Inorg Chem 1984, V23, P3922
(21) Lay, P; Inorg Chem 1987, V26, P2144 CAPLUS
(22) Massaferro, A; An Quim 1992, V88, P230 CAPLUS
(23) Nordmeyer, F; Inorg Chem 1969, V8, P2781
(24) Rotzinger, F; Inorg Chem 1988, V27, P768 CAPLUS
(25) Rotzinger, F; Inorg Chem 1988, V27, P772 CAPLUS
(26) Rotzinger, F; Inorg Chem 1991, V30, P2763 CAPLUS
(27) Sienra, B; Polyhedron 1991, V17, P2075
(28) Sienra, B; Z Anorg Allg Chem 1990, V590, P222 CAPLUS
(29) Sisley, M; Inorg Chem 1981, V20, P2799 CAPLUS
(30) Swaddle, T; Can J Chem 1977, V55, P3166 CAPLUS
(31) Tobe, M; Inorganic Reaction Mechanisms 1999
(32) Wilkins, R; Kinetics and Mechanism of Reactions of Tr
 (32) Wilkins, R; Kinetics and Mechanism of Reactions of Transition Metal
        Complexes 1991
           ANSWER 34 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
           252564-83-3 REGISTRY
Entered STN: 10 Jan 2000
RN
ED
           Zinc, bis(4,6-dimethyl-2(1H)-pyrimidinethionato-kS2)bis(2-methyl-2-
CN
           propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
           C20 H36 N6 S2 Zn
MF
 CI
           CCS
 SR
           CA
           STN Files:
                                     CA, CAPLUS
 LC
 DT.CA CAplus document type: Journal
 RL.NP Roles from non-patents: USES (Uses)
```

# Ring System Data

Analysis FA	Sequence   ES	the Rings	Ring System   Formula   RF	RID	Count
	+======-   NCNC3		+=========   C4N2	46.195.24	2

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

AN 132:36842 CA
TI Insights into sulfur vulcanization from QSPR quantitative structure-property relationships studies
AU Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, Mati
CS Flexsys America LP, Akron, OH, USA
SO Rubber Chemistry and Technology (1999), 72(2), 318-333
CODEN: RCTEA4; ISSN: 0035-9475

```
American Chemical Society, Rubber Division
PB
DT
LA
     Enalish
      39-10 (Synthetic Elastomers and Natural Rubber)
CC
     Vulcanization of styrene-butadiene rubber, as accelerated by a series of
     sulfenamides and sulfenimides prepared from various aromatic heterocyclic
     thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent
     correlations of mol. descriptors of accelerators or accelerator thiolate
     zinc complexes to the onset of cure and maximum rate of vulcanization. The
     QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted
     mechanism for the sulfurization and crosslinking reactions.
     sulfur vulcanization SBR quant structure property relationship
ST
     Molecular structure-property relationship
     Sulfidation
     Vulcanization
     Vulcanization accelerators and agents
         (insights into sulfur vulcanization from quant. structure-property relationships studies)
      Styrene-butadiene rubber, processes
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
                                                     2 7704-34-9, sulfur, uses 15670-77-6 26773-69-3
                              102-77-2
                                           4979-32-2
                  95-33-0
IT
                     15214-44-5
                                     15214-57-0
      10220-34-5
                                     38335-52-3
                                                     38818-08-5
                                                                     137376-19-3
                     37765-44-9
      36930-73-1
                      156477-90-6
                                        157993-40-3
                                                         188036-96-6
                                                                          252564-20-8
      156017-14-0
                                        252564-23-1
                                                                          252564-25-3
                       252564-22-0
                                                         252564-24-2
      252564-21-9
                                                                          252564-30-0
                       252564-27-5
                                        252564-28-6
                                                         252564-29-7
      252564-26-4
                                                                          252564-35-5
                       252564-32-2
                                        252564-33-3
                                                         252564-34-4
      252564-31-1
                                                         252564-83-3
                       252564-37-7
                                        252564-38-8
      252564-36-6
      RL: MOA (Modifier or additive use); USES (Uses)
         (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
      95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
      RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
      reagent); USES (Uses)
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
      252564-18-4P
IT
      RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
      (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property
          relationships studies)
      37143-54-7, 1-Methoxy-2-propylamine
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
      9003-55-8
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process) (styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)
                THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS (3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
```

```
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS (7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS (8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coursely and Science and Technology of Rubber 1978, P301
(14) Coran, A, Science and Technology of Rubber 1978, P301 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett J: Chem Pay 1935, V17, P125, CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS
(23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky A: Anal Chem 1994, V66, P1709 CAPLUS
 (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Chem 1996, V100, P10400 CAPLUS
 (31) Katritzky, A; J_Phys Chem 1996, V100, P10400 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research, 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J: Sulfur, Its Significance for Chemistry for the Geo-
 (39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
 and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
  (41) Milligan, B; J Chem Soc 1966, V1, P34
 (42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
  (43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
 (44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS (45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
 (46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
             CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
 (49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tetko T: J Chem Inf Comput Sci 1996, V36, P794 CAPLUS
 (60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS
 (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS
 (62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965, P53
  (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
```

(65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS ANSWER 35 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN 252564-38-8 REGISTRY RN Entered STN: 10 Jan 2000 Zincate(1-), bis(2(3H)-benzothiazolethionato-κS2)(butanoato-κO)(2-methyl-2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX ED CN C22 H26 N3 O2 S4 Zn . H MF CI CCS SR CA STN Files: CA, CAPLUS LC DT.CA CAplus document type: Journal RL.NP Roles from non-patents: USES (Uses) CRN (742046-45-3)

#### Ring System Data

Elemental	Elemental	Size of	Ring System	Laentifier	RID
Analysis	Sequence	the Rings	Formula		Occurrence
EA	ES	SZ	RF		Count
======================================	+=== <del>=====</del>  NCSC2-C6	+=======  5-6	+========   c7ns	333.521.13	2

⊕ H+

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

132:36842 CA AN Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Mati Flexsys America LP, Akron, OH, USA Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475 American Chemical Society, Rubber Division CS S0 PB Journal DT English LA 39-10 (Synthetic Elastomers and Natural Rubber) CC

```
Vulcanization of styrene-butadiene rubber, as accelerated by a series of
AB
       sulfenamides and sulfenimides prepared from various aromatic heterocyclic
       thiols and various aliphatic amines, was studied using the curemeter under
       isothermal conditions. Further studies using MOPAC_AM1 semiempirical
       quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfunization and crosslinking reactions
       mechanism for the sulfurization and crosslinking reactions.
       sulfur_vulcanization SBR quant structure property relationship
ST
       Molecular structure-property relationship
IT
       Sulfidation
       Vulcanization
       Vulcanization accelerators and agents
            (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
        Styrene-butadiene rubber, processes
IT
       RL: PEP (Physical, engineering or chemical process); PROC (Process) (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
                                                                        7704-34-9, sulfur, uses
70-77-6 26773-69-3
                                                      4979-32-2
                      95-33-0
                                      102-77-2
        95-29-4
IT
        10220-34-5
                           15214-44-5
                                               15214-57-0
                                                                  15670-77-6
                                                                                      137376-19-3
                                               38335-52-3
                                                                   38818-08-5
        36930-73-1
                           37765-44-9
                                                                                            252564-20-8
                                                  157993-40-3
                                                                       188036-96-6
        156017-14-0
                            156477-90-6
                                                                                            252564-25-3
                                                  252564-23-1
                                                                       252564-24-2
                             252564-22-0
        252564-21-9
                                                                                             252564-30-0
                                                                       252564-29-7
                                                  252564-28-6
252564-33-3
                             252564-27-5
        252564-26-4
                                                                       252564-34-4
                                                                                            252564-35-5
                             252564-32-2
        252564-31-1
                                                                       252564-83-3
                                                  252564-38-8
                             252564-37-7
        252564-36-6
        RL: MOA (Modifier or additive use); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
        95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
IT
        reagent); USES (Uses)
            (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
        252564-18-4P
IT
        RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
        (Preparation); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
        37143-54-7, 1-Methoxy-2-propylamine
IT
        RL: RCT (Reactant); RACT (Reactant or reagent) (insights into sulfur vulcanization from quant. structure-property
             relationships studies)
IT
        RL: PEP (Physical, engineering or chemical process); PROC (Process)
             (styrene-butadiene rubber, insights into sulfur vulcanization from
            quant. structure-property relationships studies)
                     THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers T: Natural 1974, V252, P32 CAPLUS
 (9) Chivers, T; Nature 1974, V252, P32 CAPLUS
```

```
(10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
 (11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS
(12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301
(14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS (22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS (24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS (25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
 (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
 (27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
   33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
34) Krebs, H; Rubber Chem Technol 1957, V30, P962
 (35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS (36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS (37) Kresja, M; Rubber Chem Technol 1993, V66, P376
 (38) Lichty, J; US 2129621 1938 CAPLUS
 (39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
 and Cosmosphere Technology 1984, V5, P31

(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115

(41) Milligan, B; J Chem Soc 1966, V1, P34

(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS

(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS

(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
  (45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
 (46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
              CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977
 (47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
(50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
(51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS
(52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS
(53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R: J Am Chem Soc 1952, V74, P3120 CAPLUS
  (58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
  (59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196 (63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
```

L9 ANSWER 36 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN

```
252564-37-7 REGISTRY
RN
     Entered STN: 10 Jan 2000
ED
     Zincate(1-), (butanoato-\kappa0)(2-methyl-2-propanamine)bis(2(1H)-
CN
     pyrimidinethionato-kS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
     C16 H24 N5 O2 S2 Zn . H
MF
CI
     CCS
SR
     CA
     STN Files:
                    CA, CAPLUS
LC
DT.CA Caplus document type: Journal RL.NP Roles from non-patents: USES (Uses)
CRN (788144-09-2)
```

# Ring System Data

EA	ES	SZ	Ring System   Formula   RF	Ring  Identifier   RID	RID Occurrence Count
		+======-   6	+=====================================	46.195.24	2

● H+

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

132:36842 CA AN Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Flexsys America LP, Akron, OH, USA CS Rubber Chemistry and Technology (1999), 72(2), 318-333 50 CODEN: RCTEA4; ISSN: 0035-9475 American Chemical Society, Rubber Division PΒ DT Journal English LA 39-10 (Synthetic Elastomers and Natural Rubber)
Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic CC AB thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate

```
zinc complexes to the onset of cure and maximum rate of vulcanization. The
      QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted
      mechanism for the sulfurization and crosslinking reactions.
      sulfur vulcanization SBR quant structure property relationship
ST
      Molecular structure-property relationship
IT
      Sulfidation
      Vulcanization
      Vulcanization accelerators and agents
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
      Styrene-butadiene rubber, processes
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
                                                                  7704-34-9, Sulfur, uses
                                  102-77-2
                                                 4979-32-2
                    95-33-0
IT
      95-29-4
                                                             15670-77-6
                                                                               26773-69-3
                        15214-44-5
                                           15214-57-0
       10220-34-5
                                           38335-52-3
                                                             38818-08-5
                                                                               137376-19-3
                         37765-44-9
       36930-73-1
                                                                                    252564-20-8
                                             157993-40-3
                                                                 188036-96-6
                          156477-90-6
       156017-14-0
                                                                                    252564-25-3
                                             252564-23-1
                                                                 252564-24-2
                          252564-22-0
       252564-21-9
                                                                 252564-29-7
                                                                                    252564-30-0
                          252564-27-5
                                             252564-28-6
       252564-26-4
                                                                 252564-34-4
                                                                                    252564-35-5
                                             252564-33-3
                          252564-32-2
       252564-31-1
                                                                 252564-83-3
                                             252564-38-8
                          252564-37-7
       252564-36-6
       RL: MOA (Modifier or additive use); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
       RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
       reagent); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
IT
       252564-18-4P
       RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
       (Preparation); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       37143-54-7, 1-Methoxy-2-propylamine
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       9003-55-8
IT
       RL: PEP (Physical, engineering or chemical process); PROC (Process) (styrene-butadiene rubber, insights into sulfur vulcanization from
           quant. structure-property relationships studies)
                   THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS (3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
 (4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substance (5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS (6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS (7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS (8) Chapman, A; Natural Rubber Science and Technology 1988, P511 (9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS (11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis. D: J Am Chem Soc 1967, V89, P1346 CAPLUS
 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS
```

```
(16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS (22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS (24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS (25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS (26) Katritzky, A: Anal Chem 1994, V66, P1799 CAPLUS
(16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS
(26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(3U) Katritzky, A; J Chem Int Comput SCI 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J: Sulfur, Its Significance for Chemistry, for the Geo-
 (39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
 (41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
 (43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
 (44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
         CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977
 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
 (49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
(50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
(51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
 (59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
 (60) Tetko, í; J Chem Inf Comput Sči 1996, V36, P794 CÁPLUS
(61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS
(62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
           ANSWER 37 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
           252564-36-6 REGISTRY
Entered STN: 10 Jan 2000
RN
ED
           Zincate(1-), (butanoato-\kappa0)(2-methyl-2-propanamine)bis(2(1H)-
CN
            pyridinethionato-kS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
MF
           C18 H26 N3 O2 S2 Zn . H
CI
           CCS
```

SR CA

STN Files: CA, CAPLUS LC

DT.CA CAplus document type: Journal RL.NP Roles from non-patents: USES (Uses)

CRN (750557-81-4)

Ring System Data

Analysis	Elemental  Sequence   ES	Size of  the Rings   SZ	Ring System   Formula   RE	Taeut II ier	RID Occurrence Count
======================================	+========   NC5	+=======-   6	C5N	46.156.21	2

● H+

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

AN

Insights into sulfur vulcanization from QSPR quantitative TI

structure-property relationships studies

Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU

CS

Flexsys America LP, Akron, OH, USA Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475 S<sub>0</sub>

American Chemical Society, Rubber Division PB

Journal DT

English LA

39-10 (Synthetic Elastomers and Natural Rubber) CC Vulcanization of styrene-butadiene rubber, as accelerated by a series of AB sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted

```
mechanism for the sulfurization and crosslinking reactions.
       sulfur vulcanization SBR quant structure property relationship
ST
       Molecular structure-property relationship
IT
       Sulfidation
       Vulcanization
       Vulcanization accelerators and agents
            (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
       Styrene-butadiene rubber, processes
IT
       RL: PEP (Physical, engineering or chemical process); PROC (Process) (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
                                                                       7704-34-9, sulfur, uses
0-77-6 26773-69-3
                     95-33-0
                                                     4979-32-2
                                    102-77-2
IT
       95-29-4
                                              15214-57-0
                                                                 15670-77-6
       10220-34-5
                          15214-44-5
                                                                                    137376-19-3
                                                                 38818-08-5
                          37765-44-9
                                              38335-52-3
       36930-73-1
                                                                                          252564-20-8
                                                 157993-40-3
                                                                     188036-96-6
                           156477-90-6
       156017-14-0
                                                                                          252564-25-3
                                                                     252564-24-2
                                                 252564-23-1
                            252564-22-0
       252564-21-9
                                                                     252564-29-7
                                                                                          252564-30-0
                            252564-27-5
                                                 252564-28-6
       252564-26-4
                           252564-32-2
252564-37-7
                                                 252564-33-3.
                                                                     252564-34-4
                                                                                          252564-35-5
       252564-31-1
                                                                     252564-83-3
                                                 252564-38-8
       252564-36-6
       RL: MOA (Modifier or additive use); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
       95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
       RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
       reagent): USES (Uses)
            (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
       252564-18-4P
IT
       RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
            (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
       37143-54-7, 1-Methoxy-2-propylamine
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
            (insights into sulfur vulcanization from quant. structure-property
            relationships studies)
       9003-55-8
IT
       RL: PEP (Physical, engineering or chemical process); PROC (Process)
            (styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)
                     THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
(1) Anon; Natural Rubber Science and Technology 1988, P570 (2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS (3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449 (5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS (6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS (7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS (8) Chapman, A; Natural Rubber Science and Technology 1988, P511 (9) Chivers T: Natural 1974, V252, P32 CAPLUS
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS
(10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS
(12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS
(13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS
(14) Coran, A; Science and Technology of Rubber 1978, P301
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS
(17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS
(19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS
```

```
(20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS (29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS (30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS (31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS (32) Kion Li Molecular Connectivity in Chemistry and David Research
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976 (33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS (34) Krebs, H; Rubber Chem Technol 1957, V30, P962 (35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS (36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS (37) Kresja, M; Rubber Chem Technol 1994, V67, P376 (38) Lighty J: US 2129621 1938 CAPLUS
 (38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-, and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
(41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
 (44) Morita, É; Rubber Chem Technol 1984, V57, P744 CAPLUS
 (45) Murugan, Ŕ; Chemtech 1994, V24(6), P17 CAPLUS
 (46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
 (47) Porter, M; The Chemistry of Sulfides 1977 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173 (54) Stanton D; Anal Chem 1990, V62, P2222 CAPLUS
(53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P1/3 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS (55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS (56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS (57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS (58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS (59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS (60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J: J Soc Rubber Ind Jon 1952, V25, P267 CAPLUS
 (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196 (63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
 (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
            ANSWER 38 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
            252564-35-5 REGISTRY
 RN
            Entered STN: 10 Jan 2000
 ED
            Zincate(1-), (butanoato-κο)(2-methyl-2-propanamine)bis(2(1H)-
            pyrazinethionato-kS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME) C16 H24 N5 O2 S2 Zn . H
CN
MF
CI
            CCS
SR
            CA
                                         CA, CAPLUS
 LC
            STN Files:
                                                                    Journal
DT.CA CAplus document type:
RL.NP Roles from non-patents: USES (Uses)
```

CRN (740072-13-3)

Ring System Data

Elemental		Size of	Ring System	Ring	RID
Analysis		the Rings	Formula	Identifier	Occurrence
EA		SZ	RF	RID	Count
======== C4N2	+=======   NC2NC2	-=========  6	C4N2	46.383.8	2

● н+

132:36842 CA

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Flexsys America LP, Akron, OH, USA CS Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475 American Chemical Society, Rubber Division SO PB DT Journal English LA 39-10 (Synthetic Elastomers and Natural Rubber) CC Vulcanization of styrene-butadiene rubber, as accelerated by a series of AB sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions. sulfur vulcanization SBR quant structure property relationship ST Molecular structure-property relationship IT

Sulfidation

```
Vulcanization
      Vulcanization accelerators and agents
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
      Styrene-butadiene rubber, processes
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
                                                                  7704-34-9, Sulfur, uses
                                                  4979-32-2
                                 102-77-2
       95-29-4
                   95-33-0
IT
                                                             15670-77-6
                                                                               26773-69-3
                                           15214-57-0
      10220-34-5
                         15214-44-5
                                           38335-52-3
                                                                               137376-19-3
                                                             38818-08-5
       36930-73-1
                         37765-44-9
                                             157993-40-3
                                                                 188036-96-6
                                                                                     252564-20-8
                          156477-90-6
       156017-14-0
                                                                                     252564-25-3
                                              252564-23-1
                                                                 252564-24-2
                          252564-22-0
       252564-21-9
                                                                 252564-29-7
                                                                                     252564-30-0
                          252564-27-5
                                              252564-28-6
       252564-26-4
                                                                 252564-34-4
                                                                                     252564-35-5
                          252564-32-2
252564-37-7
                                              252564-33-3
       252564-31-1
                                                                 252564-83-3
                                             252564-38-8
       252564-36-6
      RL: MOA (Modifier or additive use); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
      95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
       RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
       reagent); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
IT
       252564-18-4P
      RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
       (Preparation); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       37143-54-7, 1-Methoxy-2-propylamine
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       9003-55-8
TT
       RL: PEP (Physical, engineering or chemical process); PROC (Process)
           (styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)
                   THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(1) Anon; Natural Rubber Science and Technology 1300, 1370
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS
(17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall H: J Am Chem Soc 1967, V70, P6441 CAPLUS
(20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
```

```
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(27) Katritzky, A; CODESSA RETERENCE Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresia, M; Rubber Chem Technol 1993, V66, P376
 (37) Kresja, M; Rubber Chem Technol 1993, V66, P376
 (38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
and Cosmosphere Technology 1984, V5, P31

(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115

(41) Milligan, B; J Chem Soc 1966, V1, P34

(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS

(43) Moore C: J Chem Soc 1954, P2082, CAPLUS
 (43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
 (45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
          CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977
 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173 (54) Stanton D: Angl Chem 1990, V62, P2222 CAPLUS
 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS (55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
  (56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS (57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS (58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(58) Tatt, R; J Am Chem Soc 1952, V/4, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS
(61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS
(62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965, P53
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
(65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS
(66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
            ANSWER 39 OF 121 REGISTRY COPYRIGHT 2006 ACS. on STN.
            252564-34-4 REGISTRY
 RN
            Entered STN: 10 Jan 2000
 ED
            Zincate(1-), (butanoato-κο)(2-methyl-2-propanamine)bis(4-nitro-2(1H)-
 CN
            pyridinethionato-kS2)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
 MF
            C18 H24 N5 O6 S2 Zn . H
 CI
            CCS
 SR
            STN Files:
                                        CA, CAPLUS
 DT.CA CAplus document type:
                                                                     Journal
                Roles from non-patents: USES (Uses)
 CRN (774525-06-3)
```

Ring System Data

Elemental Analysis EA	Sequence   ES	the Rings	Ring System   Formula   RF	Ring Identifier RID	RID Occurrence Count
======== C5N	+======-   NC5	+========  6	C5N	46.156.21	2

$$\begin{array}{c|c}
0 \\
0 \\
\hline
0 \\
C-Pr-n
\end{array}$$

$$\begin{array}{c|c}
0 \\
\hline
0 \\
C-Pr-n
\end{array}$$

$$\begin{array}{c|c}
NO2 \\
\hline
NNO2 \\
\hline
NH2-Bu-t
\end{array}$$

● H+

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

132:36842 CA  $\Delta N$ Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Mati Flexsys America LP, Akron, OH, USA CS Rubber Chemistry and Technology (1999), 72(2), 318-333 SO. CODEN: RCTEA4; ISSN: 0035-9475 American Chemical Society, Rubber Division PB Journal DT English LA 39-10 (Synthetic Elastomers and Natural Rubber) CC Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate AB zinc complexes to the onset of cure and maximum rate of vulcanization. QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions. sulfur\_vulcanization SBR quant structure property relationship ST Molecular structure-property relationship IT Sulfidation **Vulcanization** Vulcanization accelerators and agents (insights into sulfur vulcanization from quant. structure-property relationships studies) Styrene-butadiene rubber, processes .IT

RL: PEP (Physical, engineering or chemical process); PROC (Process)

```
(insights into sulfur vulcanization from quant. structure-property
              relationships studies)
                                                                                     7704-34-9, Sulfur, uses
70-77-6 26773-69-3
                                                                4979-32-2
                                            102-77-2
IT
         95-29-4
                          95-33-0
                                                                              15670-77-6
                                                       15214-57-0
                                15214-44-5
         10220-34-5
                                                                                                      137376-19-3
                                                                              38818-08-5
                                                       38335-52-3
                                37765-44-9
         36930-73-1
                                                                                   188036-96-6
                                                                                                             252564-20-8
                                                          157993-40-3
                                 156477-90-6
         156017-14-0
                                                                                                             252564-25-3
                                                                                   252564-24-2
                                                           252564-23-1
                                 252564-22-0
         252564-21-9
                                                                                                             252564-30-0
                                                                                   252564-29-7
                                                           252564-28-6
         252564-26-4
                                 252564-27-5
                                                                                                             252564-35-5
                                                                                   252564-34-4
                                  252564-32-2
                                                           252564-33-3
         252564-31-1
                                                                                   252564-83-3
                                 252564-37-7
                                                          252564-38-8
         252564-36-6
        RL: MOA (Modifier or additive use); USES (Uses)
              (insights into sulfur vulcanization from quant. structure-property
              relationships studies)
        95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
        RL: MOA' (Modifier or additive use); RCT (Reactant); RACT (Reactant or
         reagent); USES (Uses)
              (insights into sulfur vulcanization from quant. structure-property
              relationships studies)
         252564-18-4P
IT
         RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
         (Preparation); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property
              relationships studies)
         37143-54-7, 1-Methoxy-2-propylamine
IT
         RL: RCT (Reactant); RACT (Reactant or reagent)
               (insights into sulfur vulcanization from quant. structure-property
              relationships studies)
         9003-55-8
IT
         RL: PEP (Physical, engineering or chemical process); PROC (Process) (styrene-butadiene rubber, insights into sulfur vulcanization from
              quant. structure-property relationships studies)
                         THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
              66
RE.CNT
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS (3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS
(10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS
(12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS
(13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS
(14) Coran, A; Science and Technology of Rubber 1978, P301
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS
(16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS (22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS (24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS (25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS (26) Katritzky. A: Anal Chem 1994, V66, P1799 CAPLUS
 (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
 (27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
```

```
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS

(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-, and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
(41) Milligan, B; J Chem Soc 1966. V1. P34

 (31) Katritzký, A; J Phys Chem 1996, V100, P10400 CAPLUS
 (41) Milligan, B; J Chem Soc 1966, V1, P34
 (42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS (43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
 (44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS (45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
 (46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
         CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977
 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
 (49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Shades Compute Sci 1994, V34, P382 CAPLUS
 (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tatko T: 1 Chem Inf Comput Sci 1996, V36, P794 CAPLUS
 (64) Watson, A; Steric Effects in organic Chemistry 1936, P336 (60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196 (63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wishers William Chem Sci 1947, V69, P17 CAPLUS
 (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
           ANSWER 40 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
           252564-31-1 REGISTRY
 RN
           Entered STN: 10 Jan 2000
Zincate(1-), bis(2(3H)-benzothiazolethionato-KS2)(butanoato-
 ED
 CN
           кО) (2-propanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
           C21 H24 N3 O2 S4 Zn . H
 MF
 CI
           CCS
 SR
           CA
           STN Files:
                                      CA, CAPLUS
 LC
 DT.CA CAplus document type:
                                                              Journal
 RL.NP Roles from non-patents: USES (Uses)
         (765886-51-9)
 CRN
 Ring System Data
 Elemental|Elemental| Size of |Ring System|
                                                                                                Ring
                                                                                                                       RID
                                                                                        |Identifier|Occurrence
 Analysis |Sequence |the Rings| Formula
                                                                                                               Count
                                                                        RF
                                                                                                RID
                           ES
                                          SZ
       EΑ
                                                                                       =+===============
 |333.521.13|2
 C3NS-C6 | NCSC2-C6 | 5-6
                                                              C7NS
```

$$S = S - Zn - S$$

$$S - Zn - S - S$$

$$S - Zn - S - S$$

$$S - Zn - S - S$$

H+

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

. . . .

#### REFERENCE 1

132:36842 CA Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Flexsys America LP, Akron, OH, USA CS Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475 S0 American Chemical Society, Rubber Division PΒ Journal DT English LA 39-10 (Synthetic Elastomers and Natural Rubber) CC Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic AB sultenamides and sultenimides prepared from various aromatic neterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions. mechanism for the sulfurization and crosslinking reactions. sulfur vulcanization SBR quant structure property relationship ST Molecular structure-property relationship TT **Sulfidation Vulcanization** Vulcanization accelerators and agents (insights into sulfur vulcanization from quant. structure-property relationships studies) styrene-butadiene rubber, processes IT RL: PEP (Physical, engineering or chemical process); PROC (Process) (insights into sulfur vulcanization from quant. structure-property relationships studies) 7704-34-9, sulfur, uses 70-77-6 26773-69-3 95-29-4 95-33-0 102-77-2 10220-34-5 15214-44-5 152 4979-32-2 IT 15214-44-5 15214-57-0 15670-77-6 137376-19-3 38818-08-5 38335-52-3 37765-44-9 36930-73-1

```
252564-20-8
                                                                                             188036-96-6
                                                                 157993-40-3
          156017-14-0
                                     156477-90-6
                                                                                             252564-24-2
                                                                                                                         252564-25-3
                                                                 252564-23-1
                                     252564-22-0
          252564-21-9
                                                                                             252564-29-7
                                                                                                                         252564-30-0
                                                                 252564-28-6
252564-33-3
                                     252564-27-5
          252564-26-4
                                                                                             252564-34-4
                                                                                                                         252564-35-5
                                     252564-32-2
          252564-31-1
                                                                 252564-38-8
                                                                                             252564-83-3
                                     252564-37-7
          252564-36-6
          RL: MOA (Modifier or additive use); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
IT
          reagent); USES (Uses)
                (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          252564-18-4P
IT
          RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
          (Preparation); USES (Uses)
                (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          37143-54-7, 1-Methoxy-2-propylamine
IT
          RL: RCT (Reactant); RACT (Reactant or reagent) (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          9003-55-8
IT
          RL: PEP (Physical, engineering or chemical process); PROC (Process)
                 (styrene-butadiene rubber, insights into sulfur vulcanization from
                quant. structure-property relationships studies)
                            THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman A: Natural Rubber Science and Technology 1988, P511
 (8) Chapman, A; Natural Rubber Science and Technology 1988, P511
 (9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301
(14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS (22) Hann, C: Rubber Chem Technol 1994, V67, P76 CAPLUS
 (22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
 (24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
 (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
 (27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier J: Molecular Connectivity in Chemistry and Daug Boson
(32) Kier J: Molecular Connectivity in Chemistry and Daug Boson
  (32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
 (34) Krebs, H; Rubber Chem Technol 1957, V30, P962
```

```
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS (36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS (37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
and Cosmosphere Technology 1984, V5, P31

(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115

(41) Milligan, B; J Chem Soc 1966, V1, P34

(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS

(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS

(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS

(45) Muruan B: Chemtach 1994, V24(6), P17 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
       CAPLUS
(47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
(50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
(51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS...
(52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS.
(53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196 (63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
        ANSWER 41 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
        252564-30-0 REGISTRY
RN
        Entered STN: 10 Jan 2000
ED
        Zincate(1-), bis(2(3H)-benzothiazolethionato-\kappaS2)(butanoato-
CN
        κΟ)(ethanamine)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
C20 H22 N3 O2 S4 Zn . H
MF
        CCS
CI
SR
        CA
        STN Files:
                             CA, CAPLUS
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: USES (Uses)
CRN (760160-39-2)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                                            Ring
                                                                      |Identifier|Occurrence
Analysis |Sequence | the Rings | Formula
                                                                            RID
                                                                                     Count
                                SZ
                                                         RF
     EΑ
                      ES
|333.521.13|2
                                                 C7NS
C3NS-C6 | NCSC2-C6 | 5-6
```

● H+

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

```
132:36842 CA
ΑN
      Insights into sulfur vulcanization from QSPR quantitative
TI
      structure-property relationships studies
      Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson,
ΑU
      Mati
      Flexsys America LP, Akron, OH, USA
CS
      Rubber Chemistry and Technology (1999), 72(2), 318-333
S<sub>0</sub>
      CODEN: RCTEA4; ISSN: 0035-9475
      American Chemical Society, Rubber Division
PB
DT
      English
LA
      39-10 (synthetic Elastomers and Natural Rubber)
Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic
CC
AB
      thiols and various aliphatic amines, was studied using the curemeter under
      isothermal conditions. Further studies using MOPAC_AM1 semiempirical
      quantum mech. calcns. and CODESSA QSAR software yielded excellent
      correlations of mol. descriptors of accelerators or accelerator thiolate
      zinc complexes to the onset of cure and maximum rate of vulcanization. The
      QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
      sulfur vulcanization SBR quant structure property relationship
ST
      Molecular structure-property relationship
IT
      Sulfidation
      Vulcanization
      Vulcanization accelerators and agents
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
      Styrene-butadiene rubber, processes
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
                                                         7704-34-9, Sulfur, uses
                             102-77-2
                                           4979-32-2
                 95-33-0
      95-29-4
IT
                                     15214-57-0
                                                     15670-77-6
                                                                     26773-69-3
      10220-34-5
                      15214-44-5
                                     38335-52-3
                                                     38818-08-5
                                                                     137376-19-3
                      37765-44-9
      36930-73-1
                                        157993-40-3
                                                                         252564-20-8
                       156477-90-6
                                                        188036-96-6
      156017-14-0
                                                                         252564-25-3
                                                        252564-24-2
      252564-21-9
                       252564-22-0
                                        252564-23-1
                                                                         252564-30-0
                                                        252564-29-7
                                        252564-28-6
                       252564-27-5
      252564-26-4
                                                                         252564-35-5
                                        252564-33-3
                                                        252564-34-4
                       252564-32-2
      252564-31-1
                                                        252564-83-3
                                        252564-38-8
                       252564-37-7
```

252564-36-6

```
RL: MOA (Modifier or additive use); USES (Uses)
                  (insights into sulfur vulcanization from quant. structure-property
                  relationships studies)
           95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
           RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
           reagent); USES (Uses)
                  (insights into sulfur vulcanization from quant. structure-property
                  relationships studies)
           252564-18-4P
IT
           RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
           (Preparation); USES (Uses)
                  (insights into sulfur vulcanization from quant. structure-property
                  relationships studies)
           37143-54-7, 1-Methoxy-2-propylamine
IT
           RL: RCT (Reactant); RACT (Reactant or reagent)
                  (insights into sulfur vulcanization from quant. structure-property
                  relationships studies)
IT
           9003-55-8
           RL: PEP (Physical, engineering or chemical process); PROC (Process)
                  (styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)
                               THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
                 66
(1) Anon; Natural Rubber Science and Technology 1988, P570
 (2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
 4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substance (5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS (6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS (7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS (8) Chapman, A; Natural Rubber Science and Technology 1988, P511 (9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS (11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis. D: J Am Chem Soc 1967. V89, P1346 CAPLUS
(14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS (22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS (24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS (25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
  25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
 (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
 (27) Katritzký, A; CODESSA Reference Manual 1994
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresia. M; Rubber Chem Technol 1993, V66, P376
 (37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
```

```
and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
(41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
      CAPLUS
(47) Porter, M; The Chemistry of Sulfides 1977 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
 (49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
(51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tatko T; J Chem Inf Comput Sci 1996, V36, P704 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
        ANSWER 42 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        252564-28-6 REGISTRY
RN
        Entered STN: 10 Jan 2000
ED
                            (butanoato-\kappa0)(2-methyl-2-propanamine)bis(4-methyl-
        Zincate(1-),
        2(1H)-quinolinethionato-kS2)-, hydrogen, (T-4)- (9CI) (CA INDEX
        NAME)
        C28 H34 N3 O2 S2 Zn . H
MF
CI
        CCS
SR
        CA
                          CA, CAPLUS
        STN Files:
DT.CA CAplus document type:
                                               Journal
           Roles from non-patents: USES (Uses)
RL.NP
CRN (755740-20-6)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                                       Ring
                                                                                         RID.
                                                                  |Identifier|Occurrence
Analysis |Sequence |the Rings|
                                                   Formula
                                                      RF
                                                                  | RID | Count
     EA
                     ES
                                     SZ
                            |591.79.43 |2
                                               C9N
                              6-6
C5N-C6
               NC5-C6
```

● H+

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

132:36842 CA ΑN Insights into sulfur vulcanization from QSPR quantitative ΤI structure-property relationships studies Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Mati Flexsys America LP, Akron, OH, USA Rubber Chemistry and Technology (1999), 72(2), 318-333 CS S0 CODEN: RCTEA4; ISSN: 0035-9475 American Chemical Society, Rubber Division PB Journal DT English LA 39-10 (Synthetic Elastomers and Natural Rubber) CC Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate AB zinc complexes to the onset of cure and maximum rate of vulcanization. QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions. sulfur vulcanization SBR quant structure property relationship ST Molecular structure-property relationship IT Sulfidation **Vulcanization** Vulcanization accelerators and agents (insights into sulfur vulcanization from quant. structure-property relationships studies) Styrene-butadiene rubber, processes IT RL: PEP (Physical, engineering or chemical process); PROC (Process)

(insights into sulfur vulcanization from quant. structure-property

relationships studies)

```
7704-34-9, sulfur, uses
20-77-6 26773-69-3
                              95-33-0
                                                                          4979-32-2
                                                 102-77-2
IT.
          95-29-4
                                                                                           15670-77-6
                                                               15214-57-0
          10220-34-5
                                     15214-44-5
                                                                                                                     137376-19-3
                                                                38335-52-3
                                                                                           38818-08-5
                                     37765-44-9
          36930-73-1
                                                                                                                              252564-20-8
                                                                                                 188036-96-6
                                       156477-90-6
                                                                    157993-40-3
          156017-14-0
                                                                                                                              252564-25-3
                                                                                                 252564-24-2
                                                                    252564-23-1
                                       252564-22-0
          252564-21-9
                                                                                                 252564-29-7
                                                                                                                              252564-30-0
                                                                    252564-28-6
                                       252564-27-5
          252564-26-4
                                                                    252564-33-3
                                                                                                                              252564-35-5
                                       252564-32-2
                                                                                                 252564-34-4
          252564-31-1
                                       252564-37-7
                                                                                                 252564-83-3
                                                                    252564-38-8
          252564-36-6
          RL: MOA (Modifier or additive use); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
          RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
          reagent); USES (Uses)
                 (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          252564-18-4P
IT
          RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
          (Preparation); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          37143-54-7, 1-Methoxy-2-propylamine
IT
          RL: RCT (Reactant); RACT (Reactant or reagent)
                 (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          9003-55-8
IT
          RL: PEP (Physical, engineering or chemical process); PROC (Process)
                 (styrene-butadiene rubber, insights into sulfur vulcanization from
                 quant. structure-property relationships studies)
                             THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT bb THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers. T: Nature 1974, V252, P32 CAPLUS
(8) Chapman, A; Natural Rubber Science and Technology 1988, (9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS (11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
 (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
 (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS
(23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
 (31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
```

```
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty J; US 2120621 1038 CAPLUS
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
and Cosmosphere Technology 1984, V5, P31

(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115

(41) Milligan, B; J Chem Soc 1966, V1, P34

(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS

(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS

(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
 (45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
        CAPLUS
(47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
(50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
(51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS
(52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS
(53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft R: J Am Chem Soc 1952, V74, P3120 CAPLUS
 (58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
 (59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(59) Tart, R; steric Effects in Organic Chemistry 1956, P556 (60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196 (63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
           ANSWER 43 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
           252564-27-5 REGISTRY
Entered STN: 10 Jan 2000
RN
ED
          Zinc, bis(2-methyl-2-propanamine)bis(4-methyl-2(1H)-quinolinethionato-
CN
           \kappaS2)-, (T-4)- (9CI) (CA INDEX NAME)
           C28 H38 N4 S2 Zn
MF
CI
           CCS
SR
           CA
                                     CA, CAPLUS
           STN Files:
LC
DT.CA CAplus document type: Journal
              Roles from non-patents: USES (Uses)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                                                              Rina
Analysis | Sequence | the Rings | Formula | Identifier | Occurrence
                                                                                              RID | Count
                                               SZ
                                                                      RF
       EΑ
                           ES
                                                                                    =+==================
  |591.79.43 |2
                                                             |C9N
                   NC5-C6
                                        |6-6
 C5N-C6
```

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
REFERENCE 1
```

```
132:36842 CA
AN
      Insights into sulfur vulcanization from QSPR quantitative
TI
      structure-property relationships studies
      Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson,
ΑU
      Mati
      Flexsys America LP, Akron, OH, USA
CS
      Rubber Chemistry and Technology (1999), 72(2), 318-333
SO
      CODEN: RCTEA4; ISSN: 0035-9475
      American Chemical Society, Rubber Division
PB
DT
       Journal
       English
LA
      39-10 (Synthetic Elastomers and Natural Rubber)
CC
      Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic
AB
      thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent
      correlations of mol. descriptors of accelerators or accelerator thiolate
      zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted
      mechanism for the sulfurization and crosslinking reactions.
      sulfur vulcanization SBR quant structure property relationship
ST
      Molecular structure-property relationship
IT
       Sulfidation
       Vulcanization
      Vulcanization accelerators and agents
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       Styrene-butadiene rubber, processes
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process) (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
                                                                7704-34-9, sulfur, uses
70-77-6 26773-69-3
                                                4979-32-2
                    95-33-0
                                 102-77-2
IT
       95-29-4
       10220-34-5
                                          15214-57-0
                                                           15670-77-6
                        15214-44-5
                                                                             137376-19-3
                                                           38818-08-5
                        37765-44-9
                                          38335-52-3
       36930-73-1
                                                                                  252564-20-8
                                            157993-40-3
                                                               188036-96-6
       156017-14-0
                         156477-90-6
                                                                                  252564-25-3
                                                               252564-24-2
                                            252564-23-1
                         252564-22-0
       252564-21-9
                                                               252564-29-7
                                                                                  252564-30-0
                         252564-27-5
                                            252564-28-6
       252564-26-4
                                            252564-33-3
                                                               252564-34-4
                                                                                  252564-35-5
       252564-31-1
                         252564-32-2
                         252564-37-7
                                                               252564-83-3
                                            252564-38-8
       252564-36-6
      RL: MOA (Modifier or additive use); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
```

95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide

IT

```
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
          reagent); USES (Uses)
                 (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          252564-18-4P
IT
          RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
           (Preparation); USES (Uses)
                 (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          37143-54-7, 1-Methoxy-2-propylamine
IT
          RL: RCT (Reactant); RACT (Reactant or reagent)
                 (insights into sulfur vulcanization from quant. structure-property
                 relationships studies)
          9003-55-8
IT
          RL: PEP (Physical, engineering or chemical process); PROC (Process)
                (styrene-butadiene rubber, insights into sulfur vulcanization from quant. structure-property relationships studies)
                             THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS
(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman, A: Natural Rubber Science and Technology 1988, P511
                66
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
 (9) Chivers, T; Nature 1974, V252, P32 CAPLUS
(10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301 (15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Coccion 1: 1 Am Chem Soc 1968
 (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS
(18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS
 (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS
(20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS (21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS (23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
 (31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(31) Kalfitzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, 1: Sulfur Its Significance for Chemistry for the Gas-
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-, and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
 (41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
```

```
(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, É; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
      CAPLUS
(47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
 (49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342
(50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
 (56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS (57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(58) Tatt, R; J Am Chem Soc 1952, V/4, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS
(61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS
(62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965, P53
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
(65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS
(66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
        ANSWER 44 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        252564-26-4 REGISTRY
RN
        Entered STN: 10 Jan 2000
ED
        Zincate(1-), (butanoato-\kappa0)(2-methyl-2-propanamine)bis(4(1H)-
CN
        pyrimidinethionato-kS4)-, hydrogen, (T-4)- (9CI) (CA INDEX NAME)
        C16 H24 N5 O2 S2 Zn . H
MF
        CCS
CI
SR
        CA
        STN Files:
                          CA, CAPLUS
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: USES (Uses)
CRN (767616-38-6)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                                      Ring
                                                                |Identifier|Occurrence
Analysis |Sequence |the Rings| Formula
                                                                               | Count
                              | SZ
                                                   RF
                                                                1
                                                                      RID
                    ES
     EΑ
|46.195.23 |2
              INCNC3
                             |6
                                            C4N2
C4N2
```

$$S-Z_{n}$$
 $S-Z_{n}$ 
 $S-Bu-t$ 

**∌** H<sup>+</sup>

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

132:36842 CA Insights into sulfur vulcanization from QSPR quantitative TI structure-property relationships studies Ignatz-Hoover, Fréd; Katritzky, Alan R.; Lobanov, Victor S.; Karelson, ΑU Flexsys America LP, Akron, OH, USA CS Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475 **SO** American Chemical Society, Rubber Division PΒ Journal DT English LA 39-10 (Synthetic Elastomers and Natural Rubber) CC Vulcanization of styrene-butadiene rubber, as accelerated by a series of Vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions. sulfur vulcanization SBR quant structure property relationship AB sulfur vulcanization SBR quant structure property relationship Molecular structure-property relationship ST IT **Sulfidation Vulcanization** Vulcanization accelerators and agents (insights into sulfur vulcanization from quant. structure-property relationships studies) Styrene-butadiene rubber, processes IT RL: PEP (Physical, engineering or chemical process); PROC (Process) (insights into sulfur vulcanization from quant. structure-property relationships studies) 102-77-2 4979-32-2 7704-34-9, Sulfur, uses

IT

95-29-4

95-33-0

```
26773-69-3
                                                15214-57-0
                                                                     15670-77-6
                            15214-44-5
       10220-34-5
                                                                                         137376-19-3
                                                                     38818-08-5
                            37765-44-9
                                                 38335-52-3
       36930-73-1
                                                    157993-40-3
                                                                          188036-96-6
                                                                                                252564-20-8
                             156477-90-6
       156017-14-0
                                                    252564-23-1
                                                                          252564-24-2
                                                                                                252564-25-3
                             252564-22-0
       252564-21-9
                                                                                                252564-30-0
                             252564-27-5
                                                                          252564-29-7
                                                    252564-28-6
       252564-26-4
                                                                                                252564-35-5
                                                                          252564-34-4
                             252564-32-2
                                                    252564-33-3
       252564-31-1
                                                                         252564-83-3
                             252564-37-7
                                                    252564-38-8
       252564-36-6
       RL: MOA (Modifier or additive use); USES (Uses)
            (insights into sulfur vulcanization from quant. structure-property
             relationships studies)
       95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
       RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
       reagent); USES (Uses)
             (insights into sulfur vulcanization from quant. structure-property
             relationships studies)
       252564-18-4P
IT
       RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
       (Preparation); USES (Uses) (insights into sulfur vulcanization from quant. structure-property
             relationships studies)
        37143-54-7, 1-Methoxy-2-propylamine
IT
        RL: RCT (Reactant); RACT (Reactant or reagent)
             (insights into sulfur vulcanization from quant. structure-property
             relationships studies)
        9003-55-8
IT
       RL: PEP (Physical, engineering or chemical process); PROC (Process)
             (styrene-butadiene rubber, insights into sulfur vulcanization from
             quant. structure-property relationships studies)
                     THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS (3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449 (5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS (6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS (7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS (8) Chapman, A; Natural Rubber Science and Technology 1988, P511 (9) Chivers T: Natura 1974, V252, P32 CAPLUS
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS
(18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS (19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS (20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS
(23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katnitzky, A: April Chem 1004, V66, P1700 CAPLUS
 (26) Katritzký, Á; Anal Chem 1994, V66, P1799 CAPLUS
 (27) Katritzky, A; CODESSA Reference Manual 1994
 (28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS (30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzký, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
```

```
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty J: Sulfur Technol for Chemistry
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-, and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
(41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
 (43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
         CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
 (49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS
 (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
(54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS
(57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS
(58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS
(59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS
(60) Tatto T: 1 Chem Inf Comput Sci 1996, V26, P704 CAPLUS
(60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander, K; Rubber Chem Technol 1994, V67, P196 (63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Sec 1947, V69, P17 CAPLUS
 (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
           ANSWER 45 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
           252564-24-2 REGISTRY
RN
           Entered STN: 10 Jan 2000
ED
           Zinc, bis(2(3H)-benzothiazolethionato-kS2)bis(2-propanamine)-,
CN
           (T-4)- (9CI) (CA INDEX NAME)
C20 H26 N4 S4 Zn
MF
CI
           CCS
           CA
SR
           STN Files:
                                     CA, CAPLUS
LC
DT.CA CAplus document type: Journal.
RL.NP Roles from non-patents: USES (Uses)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                                                                 Ring
                    |Sequence | the Rings | Formula | Identifier | Occurrence
Analysis
                                                                                                           Count
                                                                      RF
                                                                                         RID
                                         SZ
                     | ES
       EΑ
 |333.521.13|2
C3NS-C6 | NCSC2-C6 | 5-6
                                                               C7NS
```

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

```
132:36842 CA
AN
      Insights into sulfur vulcanization from QSPR quantitative
TI
      structure-property relationships studies
      Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson,
ΑU
      Măti
      Flexsys America LP, Akron, OH, USA
CS
      Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475
SO
      American Chemical Society, Rubber Division
PB
      Journal
DT
      English
LA
      39-10 (Synthetic Elastomers and Natural Rubber)
CC
      Vulcanization of styrene-butadiene rubber, as accelerated by a series of
AB
      sulfenamides and sulfenimides prepared from various aromatic heterocyclic
      thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical
      quantum mech. calcns. and CODESSA QSAR software yielded excellent
      correlations of mol. descriptors of accelerators or accelerator thiolate
      zinc complexes to the onset of cure and maximum rate of vulcanization. The
     QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted mechanism for the sulfurization and crosslinking reactions.
      sulfur vulcanization SBR quant structure property relationship
ST
      Molecular structure-property relationship
TT
      Sulfidation
      Vulcanization
      Vulcanization accelerators and agents
          (insights into sulfur vulcanization from quant. structure-property relationships studies)
      Styrene-butadiene rubber, processes
IT
      RL: PEP (Physical, engineering or chemical process); PROC (Process)
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
                                                         7704-34-9, sulfur, uses
70-77-6 26773-69-3
                                           4979-32-2
                              102-77-2
                  95-33-0
IT
                                     15214-57-0
                                                     15670-77-6
                     15214-44-5
      10220-34-5
                                                     38818-08-5
                                                                    137376-19-3
                     37765-44-9
156477-90-6
                                     38335-52-3
      36930-73-1
                                                        188036-96-6
                                                                         252564-20-8
                                        157993-40-3
      156017-14-0
                                                        252564-24-2
                                                                         252564-25-3
                                        252564-23-1
                       252564-22-0
      252564-21-9
                                        252564-28-6
                                                        252564-29-7
                                                                         252564-30-0
                       252564-27-5
      252564-26-4
                                                                         252564-35-5
                                                        252564-34-4
                       252564-32-2
      252564-31-1
                                        252564-33-3
                                                        252564-83-3
                       252564-37-7
                                        252564-38-8
      252564-36-6
      RL: MOA (Modifier or additive use); USES (Uses)
          (insights into sulfur vulcanization from quant. structure-property
          relationships studies)
      95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
```

```
RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
          reagent); USES (Uses)
                (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          252564-18-4P
IT
          RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
                (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          37143-54-7, 1-Methoxy-2-propylamine
IT
          RL: RCT (Reactant); RACT (Reactant or reagent)
                (insights into sulfur vulcanization from quant. structure-property
                relationships studies)
          9003-55-8
IT
          RL: PEP (Physical, engineering or chemical process); PROC (Process)
                (styrene-butadiene rubber, insights into sulfur vulcanization from
               quant. structure-property relationships studies)
                           THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
KE.CNI OD THEKE ARE OD CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Anon; Natural Rubber Science and Technology 1988, P570

(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS

(3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS

(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449

(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS

(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS

(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS

(8) Chapman, A: Natural Rubber Science and Technology 1988, P511
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS (10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS (12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS (13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS (16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS (17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS
 (18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS
(19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS
(20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS
(23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky A: Apal Chem 1994, V66, P1709 CAPLUS
 (26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
 (28) Katritzký, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS (30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
 (31) Katritzký, A; J Phys Chem 1996, V100, P10400 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS
(37) Kresja, M; Rubber Chem Technol 1993, V66, P376
(38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty J; Sulfur, Its Significance for Chemistry, for the Geo-
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
        and Cosmosphere Technology 1984, V5, P31
(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115
 (41) Milligan, B; J Chem Soc 1966, V1, P34
(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS
```

```
(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS
(44) Morita, É; Rubber Chem Technol 1984, V57, P744 CAPLUS
(45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
        CAPLUS
(47) Porter, M; The Chemistry of Sulfides 1977
(48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS (51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173 (54) Stanton D: Angl Chem 1990, V62, P2222 CAPLUS
(53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P1/3 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS (55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS (56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS (57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS (58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS (59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS (60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander. K: Rubber Chem Technol 1994, V67, P196
(62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965, P53
(64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS
(65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS
(66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
           ANSWER 46 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
           210574-34-8 REGISTRY
RN
           Entered STN: 30 Aug 1998
ED
           Cobalt(1+), tetraammine(methanamine)[sulfato(2-)-\kappa0]-, (OC-6-23)-
CN
                        (CA INDEX NAME)
           (9CI)
           C H17 CO N5 O4 S
MF
           CCS, COM
CI
SR
           STN Files:
                                      CA, CAPLUS
LC
              CAplus document type:
                                                               Journal
DT.CA
               Roles from non-patents: PROC (Process); PRP (Properties); RACT
RL.NP
               (Reactant or reagent)
             NH2-Me
                   _ NH3
H3N
            Co 3+
                      NH3
H<sub>3</sub>N′
             o<del>−</del> so₃−
                                 3 REFERENCES IN FILE CA (1907 TO DATE)
                                 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
```

Activation volumes for a series of spontaneous, acid-and base-catalysed

aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-, Br-,

TT

137:84151 CA

NO3-, SO42-)

```
Benzo, Fabian; Gonzalez, Gabriel; Martinez, Manuel; Sienra, Beatriz
Catedra de Quimica Inorganica, Facultad de Quimica, Universidad de la
ΑU
CS
        Republica, Montevideo, 11800, Urug.
        Inorganic Reaction Mechanisms (Amsterdam, Netherlands) (2001), 3(1), 25-29
SO.
        CODEN: IRMEFE; ISSN: 1028-6624
        Gordon & Breach Science Publishers
        Journal
DT
        English
LA
        67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
        Section cross-reference(s): 78
        The vols. of activation for the spontaneous, base-, and acid- catalyzed
AB
        path of the hydrolysis reaction of a series of trans-[Co(MeNH2)(NH3)4X](3-
       path of the hydrolysis reaction of a series of trans-[Co(MeNH2)(NH3)4X](3-n)+ ions (X = Cl-, Br-, (ONO2)- (OSO3)2-) have been determined in order to establish analogies with the dissociative trends found in previous work with the spontaneous hydrolysis of neutral ligands from the same cores. While for the base catalyzed path a significant decrease in the activation volume is found on going from the {Co(NH3)5} to the trans-{Co(MeNH2)(NH3)4} inert skeleton (i.e. 9.8, 12.5, 4.0 and 9.1 cm3mol-1 for the chloro, bromo, nitrato and sulfato derivs.), no significant changes are observed for the same complexes in the spontaneous reaction. The trends are rationalized in terms of the important changes occurring in electrostriction factors for the DCB and Id intimate mechanisms operating and the important increase in the degree of dissociativeness due to the
        and the important increase in the degree of dissociativeness due to the
        presence of a trans-methylamino ligand. For the acid catalyzed path the
        differences are much more difficult to assess, specially taking into account the limited information available as well as the inherent errors
        involved in the rate constant determination
        acid_catalyzed aquation anionic_cobalt_complex activation vol; base
ST
        catalyzed aquation anionic cobalt complex activation vol
        Activation volume
IT
        Aquation
        Aquation catalysts
        Electrostriction
              (activation vols. for a series of spontaneous, acid-and_base-catalyzed
             aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-,
        Br-, NO3-, SO42-))
Acids, uses
IT
        Bases, uses
        RL: CAT (Catalyst use); USES (Uses)
             (activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-,
              Br-, NO3-, SO42-))
        Transition metal complexes RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant
IT
              (activation vols. for a series of spontaneous, acid-and base-catalyzed
             aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-,
              Br-, NO3-, SO42-))
        36527-86-3 134066-27-6 134066-30-1 210574-34-8 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant
IT
        or reagent)
             (activation vols. for a series of spontaneous, acid-and base-catalyzed aquation reactions of trans-[Co(MeNH2)(NH3)4X]2,1+ complexes (X=Cl-,
              Br-, NO3-, SO42-))
                       THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
 (1) Balt, S; Transition Met Chem 1984, V9, P224 CAPLUS
 (2) Benzo, F; J Chem Soc 1999, P3973 CAPLUS
 (3) Benzo, F; Polyhedron 1996, V15, P1915 CAPLUS
 (4) Dixon, N; Inorg Chem 1982, V21, P688 CAPLUS
```

```
(5) Drljaca, A; Chem Rev 1998, V98, P2176
(6) Geue, R; J Am Chem Soc 1984, V106, P5478 CAPLUS (7) Gonzalez, G; J Chem Soc 1995, P891 CAPLUS (8) Kitamura, Y; Inorg Chem 1984, V23, P2038 CAPLUS (9) Lawrance, G; Inorg Chem 1984, V23, P3922 CAPLUS (10) Perrin, D; Aust J Chem 1963, V16, P372 (11) Potzinger F: Thora Chem 1989, V27, P372 (12)
(11) Rotzinger, F; Inorg Chem 1988, V27, P772 CAPLUS (12) Rotzinger, F; Inorg Chem 1991, V30, P2763 CAPLUS
(13) Tobe, M; Inorganic Reaction Mechanisms 1999
(14) Van Eldik, R; Chem Rev 1989, V89, P549 CAPLUS
(15) Van Eldik, R; Inorganic High Pressure Chemistry; Kinetics and Mechanisms
      1986
(16) Wilkins, R; Kinetics and Mechanisms of Reactions of Transition Metal
      Complexes 1991
REFERENCE 2
        133:49533 CA
AN
        Aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatocobal
TI
        t(III) complex ion
        Benzo, Fabian; Capparelli, Alberto L.; Martire, Daniel O.; Sienra, Beatriz
ΑU
        Catedra de Quimica Inorganica, Facultad de Quimica, Montevideo, C.C.1157,
CS
        Inorganic Reaction Mechanisms (Amsterdam) (2000), 1(4), 319-324
S0
        CODEN: IRMEFE; ISSN: 1028-6624
        Gordon & Breach Science Publishers
PB
        Journal
DT
        English
LA
        67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
        Section cross-reference(s): 78
        The kinetics of aquation and base hydrolysis reactions of trans-[Co(NH3)4(NH2CH3)(OSO3)]+ have been studied. In acid solution the
AB
        aquation rate, Raq, follows the equation Raq/[complex] = ks + kc[H+], at constant ionic strength \mu = 1.0 M. The activation parameters are \DeltaHs# = 88.8 kJ mol-1, \DeltaSs# = -50.5 JK-1 mol-1, \DeltaHc# =
        96.7 kJ mol-1 and \triangleSc# = -23 JK-1 mol-1. The rate consts. at 25°C are ks = 4.15 + 10-6 s-1 and kc = 4.52 M-1 s-1. The rate of base hydrolysis, ROH, follows the equation ROH/[complex] = kOH
       [OH-]. The activation parameters are \triangle HOH\# = 74.9 \text{ kJmol-1} and \triangle SOH\# = 2JK-1 \text{ mol-1} and the rate constant is kOH = 0.58 \text{ M-1 s-1} at 25°C and \mu = 0.15 \text{ M}. The stereochem. of the hydroxo product has been determined (cis-[Co(NH3)4(NH2CH3)-(OH)]2+ = 9%). The results are discussed in the light of the reaction mechanisms proposed so far.
        aquation kinetics mechanism ammine methylamine sulfato cobalt complex ion
ST
        Activation enthalpy
        Activation entropy
        Aquation kinetics
             (aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatoc
             obalt(III) complex ion)
IT
        Hydrolysis
             (base, mechanism; aquation and base hydrolysis of trans-
             tetraammine(methylamine)sulfatocobalt(III) complex ion)
        Hydrolysis kinetics
TT
             (base; aquation and base hydrolysis of trans-
             tetraammine(methylamine)sulfatocobalt(III) complex ion)
        Aquation
IT
             (mechanism; aquation and base hydrolysis of trans-
             tetraammine(methylamine)sulfatocobalt(III) complex ion)
        210574-34-8
IT
        RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
         (Reactant); PROC (Process); RACT (Reactant or reagent)
```

```
(aquation and base hydrolysis of trans-tetraammine(methylamine)sulfatoc
                      obalt(III) complex ion)
                                     THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
 (1) Adamson, A; Acta Chim Scand 1955, V9, P1261 CAPLUS
(2) Balt, S; Trans Met Chem 1984, V9, P224 CAPLUS
(2) Bail, S, Irais Met Chem 1904, V9, F224 CAPLUS
(3) Basolo, F; Mechanisms of Inorganic Reactions, 2nd edn 1
(4) Benzo, F; J Chem Crystallography 1998, V28, P69 CAPLUS
(5) Benzo, F; Polyhedron 1996, V15, P1915 CAPLUS
(6) Benzo, F; Polyhedron 1998, V17, P2295 CAPLUS
(7) Brasch, N; Inorg Chem 1989, V28, P4567 CAPLUS
(8) Buckingham, D; Inorg Chem 1970, V9, P1790 CAPLUS
(9) Buckingham, D; Inorg Chem 1970, V9, P655 CAPLUS
(10) Buckingham, D; J Am Chem Soc 1967, V89, P5129 CAPLUS
(11) Curtis, N; Inorg Chem 1986, V25, P1033 CAPLUS
(12) Curtis, N; Inorg Chem 1986, V25, P484 CAPLUS
(13) Curtis, N; Inorg Chem 1989, V28, P329 CAPLUS
(14) Dixon, N; Inorg Chem 1982, V21, P688 CAPLUS
(15) Edwards, J; Inorg Chem 1982, V21, P688 CAPLUS
(16) Finholt, J; Inorg Chem 1967, V6, P1533 CAPLUS
(17) House, D; Coord Chem Rev 1977, V23, P223 CAPLUS
(18) Jackson, W; Inorg Chem 1984, V23, P2473 CAPLUS
(19) Jackson, W; Inorg Chem 1984, V23, P668 CAPLUS
(20) Jordan, R; Inorg Chem 1984, V23, P668 CAPLUS
(21) Kitamura, Y; Inorg Chem 1989, V28, P333 CAPLUS
(22) Lawrence, G; Inorg Chem 1984, V23, P3922
(23) Lay, P; Coord Chem Rev 1991, V110, P213 CAPLUS
 (3) Basolo, F; Mechanisms of Inorganic Reactions, 2nd edn 1967
  (23) Lay, P; Coord Chem Rev 1991, V110, P213 CAPLUS (24) Lay, P; Inorg Chem 1987, V26, P2144 CAPLUS
  (25) Monacelli, F; Inorg Chim Acta 1973, V7, P65 CAPLUS
  (26) Nordmeyer, F; Inorg Chem 1969, V8, P2781
(27) Po, L; Inorg Chem 1968, V7, P526 CAPLUS
 (28) Rotzinger, F; Inorg Chem 1988, V27, P768 CAPLUS
(29) Rotzinger, F; Inorg Chem 1988, V27, P772 CAPLUS
(30) Rotzinger, F; Inorg Chem 1981, V30, P2763 CAPLUS
(31) Sisley, M; Inorg Chem 1981, V20, P2799 CAPLUS
(32) Swaddle, T; Comments Inorg Chem 1991, V12, P237 CAPLUS
(33) Taube, H; J Am Chem Soc 1953, V75, P1463 CAPLUS
(34) Tobe M: Advances in Inorganic and Riginorganic Mechans
  (34) Tobe, M; Advances in Inorganic and Bioinorganic Mechanisms 1983, V2, P1
            CAPLUS
  REFERENCE 3
               Competition study for the base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+
  ΑN
  TI
              Benzo, Fabian; Mendoza, Carolina; Queirolo, Marcelo; Sienra, Beatriz Quimica Inorganica, Facultad de Quimica, Montevideo, Urug. Polyhedron (1998), 17(13-14), 2295-2299 CODEN: PLYHDE; ISSN: 0277-5387 Elsevier Science Ltd.
  ΑU
  CS
  50
  PB
                Journal
  DT
               English
               67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
  LA
  CC
               Section cross-reference(s): 78
               Nitrite ion competition has been measured for the base hydrolysis reaction
               of trans-Co(N-H3)4(NH2CH3)Xn+ ions (X = Cl-, Br-, NO3- and SO42-) in 1.0 M NaNO2 at 25°C. Both 0- and N- bonded Co(NH3)4(NH2CH3)NO22+ are formed. Subsequently the Co(NH3)4(NH2CH3)ONO2+ isomer rearranges in OH-
  AB
               to give the thermodynamically more stable Co(NH3)4(NH2CH3)NO22+ ion. The
               total NO2- captured shows a slight dependence on the overall charge of the complex and on the nature of X (R = 2.2, 2.1, 3.6 and 1.2\pm0.5% for X = Cl-, Br-, NO3- and SO42-, resp.). These results differ from those observed
```

```
with complexes of the type Co(NH3)5Xn+ and Co(NH2CH3)5Xn+ where X includes
        a variety of anions.
        base hydrolysis kinetics cobalt ammine complex
ST
        Hydrolysis
IT
        Hydrolysis kinetics
             (base; competition study for base hydrolysis of trans-
             [Co(NH3)4(NH2CH3)X]n+ complexes)
                                                                                                         134066-30-1
                                                             36527-86-3
                                                                                  134066-27-6
        14797-65-0, Nitrite, reactions
IT
        210574-34-8
        RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
             (competition study for base hydrolysis of trans-[Co(NH3)4(NH2CH3)X]n+
             complexes)
                      THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
             22
RE.CNT
(1) Balt, S; Trans Met Chem 1984, V9, P224 CAPLUS (2) Benzo, F; Polyhedron 1996, V15, P1915 CAPLUS
(3) Benzo, F; Unpublished work
(4) Birus, M; Proc Int Conf Coord Chem 1974, V16, P3.6
(5) Bozoglian, F; Unpublished work
(6) Brasch, N; Inorg Chem 1989, V28, P4567 CAPLUS
(7) Buckingham, D; Inorg Chem 1970, V9, P1790 CAPLUS
(8) Buckingham, D; Inorg Chem 1970, V9, P655 CAPLUS
(9) Buckingham, D; Inorg Chem 1981, V20, P1647 CAPLUS
(10) Buckingham, D; J Am Chem Soc 1966, V88, P5443 CAPLUS
(11) Curtis N: Tropg Chem 1986, V25, P484 CAPLUS
(11) Curtis, N; Inorg Chem 1986, V25, P484 CAPLUS (12) Dixon, N; Inorg Chem 1982, V21, P688 CAPLUS
 (13) Haim, A; Inorg Chem 1963, V2, P1199 CAPLUS
(14) Jackson, G; Inorg Chem 1980, V19, P904
(14) Jackson, G; Inorg Chem 1980, V19, P904
(15) Jackson, W; Inorg Chem 1983, V22, P1013 CAPLUS
(16) Jackson, W; Inorg Chem 1984, V23, P2473 CAPLUS
(17) Jackson, W; Inorg Chem 1984, V23, P668 CAPLUS
(18) Massaferro, A; An Quim 1992, V88, P230 CAPLUS
(19) Rotzinger, F; Inorg Chem 1988, V27, P772 CAPLUS
(20) Rotzinger, F; Inorg Chem 1991, V30, P2763 CAPLUS
(21) Sienra, B; Z anorg allg Chem 1990, V590, P222 CAPLUS
(22) Tobe, M: Advances in Inorganic and Riginorganic Mechanic
 (22) Tobe, M; Advances in Inorganic and Bioinorganic Mechanisms 1983, V2, P1
       CAPLUS
        ANSWER 47 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
        202406-49-3 REGISTRY
RN
        Entered STN: 11 Mar 1998
ED
        Nickelate(2-), bis(methanamine)bis[sulfato(2-)-\kappa0]-, dihydrogen,
CN
        hexahydrate (9CI) (CA INDEX NAME)
C2 H10 N2 Ni 08 S2 . 6 H2 O . 2 H
MF
        CCS
CI
SR
        CA
LC
        STN Files:
                             CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties)
CRN (791764-59-5)
```

●2 H+

●6 H20

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

128:146849 CA AN Infrared and Raman spectra of Na2Cu(SO4)2.2H2O and TI (CH3NH3)2M(II)(SO4)2.6H2O with M(II) = Cu, Zn, and Ni Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B. Department of Physics, St. Gregorios College, Kottarakara, 691531, India Journal of Solid State Chemistry (1997), 133(2), 407-415 ΑU CS S0 CODEN: JSSCBI; ISSN: 0022-4596 Academic Press PB Journal DT English LA 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related CC Properties) FTIR and Raman spectra of Na2Cu(SO4)2.2H2O and FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2·6H2O > (CH3NH3)2Ni (SO4)2·6H2O > (CH3NH3)2Zn(SO4)2·6H2O > Na2Cu(SO4)2·2H2O. The appearance of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and SO42- groups. The AB the free ion indicates hydrogen bonds between NH3 and SO42- groups. The appearance of multiple bands in the bending and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2 2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mols. in (CH3NH3)2Cu(SO4)2·6H2O and (CH3NH3)2 Zn(SO4)2·6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2·6H2O.

IR Raman spectra metal sulfate hydrate; copper sodium sulfate dihydrate ST vibrational spectra; transition metal methylammonium sulfate hexahydrate; zinc methylammonium disulfate hexahydrate vibrational spectra; nickel methylammonium disulfate hexahydrate vibrational spectra Hydrogen bond IT (intramol.; in transition metal methylammonium sulfate hexahydrates

studied with vibrational spectra)

```
IR spectra
IT
          Molecular vibration
          Raman spectra
          Vibrational spectra
                 (of copper sodium sulfate dihydrate and transition metal methylammonium
                sulfate hexahydrates)
          Transition metal salts
IT
          RL: PEP (Physical, engineering or chemical process); PRP (Properties);
          PROC (Process)
                 (vibrational spectra of copper, zinc, and nickel methylammonium sulfate
                 hexahydrates)
          18901-72-9, Copper sodium sulfate (CuNa2(SO4)2) dihydrate
                                                                                                                                           202406-41-5,
IT
          Copper sodium sulfate (CuNa2(SO4)2) dideuterate
          RL: PEP (Physical, engineering or chemical process); PRP (Properties);
           PROC (Process)
                 (IR and Raman spectra and internal vibrational mode assignments)
                                        202406-47-1
                                                                      202406-49-3
          202406-44-8
IT
          RL: PEP (Physical, engineering or chemical process); PRP (Properties);
          PROC (Process)
                 (IR and Raman spectra, internal vibrational mode assignments, and
                 hydrogen bonding)
32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
(1) Abraham, S; J Raman Spectrosc 1991, V22, P245 CAPLUS
(2) Bachman, H; Naturwiss 1960, V47, P177
(3) Baran, J; J Mol Struct 1987, V162, P211 CAPLUS
(4) Bellanato, J; Spectrochim Acta 1960, V16, P1344 CAPLUS
(5) Campbell, J; Spectrochim Acta A 1970, V26, P2351 CAPLUS
(6) Dahlman, B; Ank Min 1952, V1, P220, CAPLUS
(6) Dahlman, B; Ark Min 1952, V1, P339 CAPLUS
(7) Fateley, W; Infrared and Raman Selection Rules for Molecular and Lattice
Vibrations - The Correlation Method 1972
(8) Gattow, G; Act Crystallogr 1958, V11, P377 CAPLUS
(9) Gattow, G; Acta Crystallogr 1958, V11, P866 CAPLUS
(10) Gupta, S; J Mol Struct 1984, V112, P41 CAPLUS
(11) Herzberg, G; Infrared and Raman Spectra of Polyatomic Molecules 1966
(12) Hofmann, Z; Krist 1930, V75, P158
(13) Hofmann, Z; Krist 1931, V78, P279
(14) Ikawa, S; J Raman Spectrosc 1977, V6, P89 CAPLUS
(15) Jayakumar, V; Phys Status Solid 1988, V109, P635 CAPLUS
(16) Jordanovska, V; J Therm Anal 1992, V38, P1563 CAPLUS
(17) Kamoun, M; Spectrochim Acta A 1988, V44, P471
(18) Leone. M: Period Miner 1954, V23, P223 CAPLUS
         vibrations - The Correlation Method 1972
(18) Leone, M; Period Miner 1954, V23, P223 CAPLUS
(18) Leone, M; Period Miner 1954, V23, P223 CAPLUS
(19) Mathew, X; Ph D thesis, Chap 8, University of Kerala 1989
(20) Mazzi, F; Acta Crystallogr 1955, V8, P137 CAPLUS
(21) Montgomery, H; Acta Crystallogr 1966, V20, P659 CAPLUS
(22) Montgomery, H; Acta Crystallogr 1966, V20, P728 CAPLUS
(23) Mylrajan, M; J Raman Spectrosc 1985, V16, P412 CAPLUS
(24) Nakagawa, I; Spectrochim Acta A 1964, V20, P429 CAPLUS
(25) Rajagopal, P; J Raman Spectrosc 1988, V19, P407
(26) Rama Rao, V; Acta Crystallogr 1961, V14, P738
(27) Rao, C; Chemical Applications of Infrared Spectroscopy 1963
(28) Sekar, G: J Solid State Chem 1987, V66, P235 CAPLUS
(28) Sekar, G; J Solid State Chem 1987, V66, P235 CAPLUS
(29) Sekar, G; J Solid State Chem 1988, V74, P424 CAPLUS
(30) Srinivasan, T; J Raman Spectrosc 1992, V23, P21 CAPLUS
(31) Srinivasan, T; Phase Transit 1992, V38, P97 CAPLUS
(32) Srivastava, J; J Phys C Solid State Phys 1988, V21, P4669 CAPLUS
           ANSWER 48 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN 202406-47-1 REGISTRY
L9
RN
           Entered STN: 11 Mar 1998
ED
           Zincate(2-), bis(methanamine)bis[sulfato(2-)-\kappa0]-, dihydrogen,
CN
           hexahydrate (T-4)- (9CI) (CA INDEX NAME)
```

MF C2 H10 N2 O8 S2 Zn . 6 H2 O . 2 H
CI CCS
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties)
CRN (745776-79-8)

●2 H+

●6 H<sub>2</sub>O

128:146849 CA

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

AN

Infrared and Raman spectra of Na2Cu(SO4)2  $\cdot$ 2H2O and (CH3NH3)2M(II)(SO4)2  $\cdot$ 6H2O with M(II) = Cu, Zn, and Ni TI Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B. Department of Physics, St. Gregorios College, Kottarakara, 691531, India Journal of Solid State Chemistry (1997), 133(2), 407-415 ΑU SO CODEN: JSSCBI: ISSN: 0022-4596 Academic Press PB DT Journal English LA 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related CC Properties) FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and AB  $(CH3NH3)2M(II)(SO4)2 \cdot 6H2O$  with M(II) = Cu, Zn, and Ni are recorded and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the SO42- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the SO42- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2.6H2O > (CH3NH3)2Ni (SO4)2.6H2O > (CH3NH3)2Zn(SO4)2·6H2O > Na2Cu(SO4)2·2H2O. The appearance of NH3 stretching modes at wavenumbers lower than the values obtained for the free ion indicates hydrogen bonds between NH3 and SO42- groups. The appearance of multiple bands in the bending and rocking mode regions and the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of stretching modes to lower wavenumbers and bending modes to higher stretching modes to lower wavenumbers and bending modes to higher wavenumbers of water mols. confirms the existence of strong hydrogen bonds in the crystal which is in agreement with the x-ray data. Bands indicate strong hydrogen bonds involving water mols. in

```
(CH3NH3)2Cu(SO4)2.6H2O and (CH3NH3)2 Zn(SO4)2.6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2.6H2O.
        IR Raman spectra metal sulfate hydrate; copper sodium sulfate dihydrate
ST
        vibrational spectra; transition metal methylammonium sulfate hexahydrate; zinc methylammonium disulfate hexahydrate vibrational spectra; nickel
        methylammonium disulfate hexahydrate vibrational spectra
        Hydrogen bond
IT
             (intramol.; in transition metal methylammonium sulfate hexahydrates
             studied with vibrational spectra)
IT
        IR spectra
        Molecular vibration
        Raman spectra
        Vibrational spectra
             (of copper sodium sulfate dihydrate and transition metal methylammonium
             sulfate hexahydrates)
        Transition metal salts
IT
        RL: PEP (Physical, engineering or chemical process); PRP (Properties);
        PROC (Process)
             (vibrational spectra of copper, zinc, and nickel methylammonium sulfate
             hexahydrates)
        18901-72-9, Copper sodium sulfate (CuNa2(SO4)2) dihydrate
                                                                                                          202406-41-5.
IT
        Copper sodium sulfate (CuNa2(SO4)2) dideuterate
        RL: PEP (Physical, engineering or chemical process); PRP (Properties);
        PROC (Process)
             (IR and Raman spectra and internal vibrational mode assignments)
                                                     202406-49-3
                               202406-47-1
        202406-44-8
IT
        RL: PEP (Physical, engineering or chemical process); PRP (Properties);
        PROC (Process)
             (IR and Raman spectra, internal vibrational mode assignments, and
             hydrogen bonding)
                       THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
(1) Abraham, S; J Raman Spectrosc 1991, V22, P245 CAPLUS (2) Bachman, H; Naturwiss 1960, V47, P177 (3) Baran, J; J Mol Struct 1987, V162, P211 CAPLUS
(4) Bellanato, J; Spectrochim Acta 1960, V16, P1344 CAPLUS
(5) Campbell, J; Spectrochim Acta A 1970, V26, P2351 CAPLUS
(6) Dahlman, B; Ark Min 1952, V1, P339 CAPLUS
(7) Fateley, W; Infrared and Raman Selection Rules for Molecular and Lattice
       Vibrations - The Correlation Method 1972
(8) Gattow, G; Act Crystallogr 1958, V11, P377 CAPLUS (9) Gattow, G; Acta Crystallogr 1958, V11, P866 CAPLUS (10) Gupta, S; J Mol Struct 1984, V112, P41 CAPLUS
(11) Herzberg, G; Infrared and Raman Spectra of Polyatomic Molecules 1966 (12) Hofmann, Z; Krist 1930, V75, P158 (13) Hofmann, Z; Krist 1931, V78, P279
(13) Hofmann, Z; Krist 1931, V78, P279
(14) Ikawa, S; J Raman Spectrosc 1977, V6, P89 CAPLUS
(15) Jayakumar, V; Phys Status Solid 1988, V109, P635 CAPLUS
(16) Jordanovska, V; J Therm Anal 1992, V38, P1563 CAPLUS
(17) Kamoun, M; Spectrochim Acta A 1988, V44, P471
(18) Leone, M; Period Miner 1954, V23, P223 CAPLUS
(19) Mathew, X; Ph D thesis, Chap 8, University of Kerala 1989
(20) Mazzi, F; Acta Crystallogr 1955, V8, P137 CAPLUS
(21) Montgomery, H; Acta Crystallogr 1966, V20, P659 CAPLUS
(22) Montgomery, H; Acta Crystallogr 1966, V20, P728 CAPLUS
(23) Mylrajan, M; J Raman Spectrosc 1985, V16, P412 CAPLUS
(24) Nakagawa, I; Spectrochim Acta A 1964, V20, P429 CAPLUS
(25) Rajagopal, P; J Raman Spectrosc 1988, V19, P407
(26) Rama Rao, V; Acta Crystallogr 1961, V14, P738
(26) Rama Rao, V; Acta Crystallogr 1961, V14, P738
(27) Rao, C; Chemical Applications of Infrared Spectroscopy 1963
(28) Sekar, G; J Solid State Chem 1987, V66, P235 CAPLUS (29) Sekar, G; J Solid State Chem 1988, V74, P424 CAPLUS
```

(30) Srinivasan, T; J Raman Spectrosc 1992, V23, P21 CAPLUS
(31) Srinivasan, T; Phase Transit 1992, V38, P97 CAPLUS
(32) Srivastava, J; J Phys C Solid State Phys 1988, V21, P4669 CAPLUS ANSWER 49 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN 202406-44-8 REGISTRY
Entered STN: 11 Mar 1998
Cuprate(2-), bis(methanamine)bis[sulfato(2-)-k0]-, dihydrogen,
hexahydrate (9CI) (CA INDEX NAME)
C2 H10 Cu N2 08 S2 . 6 H2 O . 2 H RN ED CN MF CI CCS CA SR CA, CAPLUS STN Files: LC DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PROC (Process); PRP (Properties) CRN (742042-77-9)

●2 H+

●6 H<sub>2</sub>O

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

128:146849 CA AN Infrared and Raman spectra of Na2Cu(SO4)2.2H2O and TI  $(CH3NH3)2M(II)(SO4)2 \cdot 6H2O$  with M(II) = Cu, Zn, and Ni Pillai, V. P. Mahadevan; Nayar, V. U.; Jordanovska, V. B. Department of Physics, St. Gregorios College, Kottarakara, 691531, India ΑU CS Journal of Solid State Chemistry (1997), 133(2), 407-415 SO CODEN: JSSCBI; ISSN: 0022-4596 Academic Press PB DT Journal English LA 73-3 (Optical, Electron, and Mass Spectroscopy and Other Related CC Properties) FTIR and Raman spectra of Na2Cu(SO4)2·2H2O and (CH3NH3)2M(II)(SO4)2·6H2O with M(II) = Cu, Zn, and Ni are recorded AB and analyzed. Bands are assigned from SO42-, CH3NH3+, and H2O vibrations. The lifting of degeneracies of v2, v3, and v4 modes and the appearance of v1 and v2 modes in the IR spectra confirm the lowering of symmetry of the 5042- ion from Td to C1 in all of the title compds. Bands obtained indicate that the distortion of the S042- ion in the four crystals are in the order, (CH3NH3) Cu(SO4)2·6H2O > (CH3NH3)2Ni (SO4)2·6H2O > (CH3NH3)2Zn(SO4)2.6H2O > Na2Cu(SO4)2.2H2O. The appearance

ST

IT

IT

IT

IT

IT

```
of NH3 stretching modes at wavenumbers lower than the values obtained for
      the free ion indicates hydrogen bonds between NH3 and SO42- groups.
      appearance of multiple bands in the bending and rocking mode regions and
      the broad nature of stretching modes show the existence of at least two sym. inequivalent water mols. in Na2Cu(SO4)2·2H2O. The shifting of
      stretching modes to lower wavenumbers and bending modes to higher
      wavenumbers of water mols. confirms the existence of strong hydrogen bonds
      in the crystal which is in agreement with the x-ray data. Bands indicate
      strong hydrogen bonds involving water mols. in (CH3NH3)2Cu(SO4)2.6H2O and (CH3NH3)2 Zn(SO4)2.6H2O and of lesser strength in (CH3NH3)2Ni(SO4)2.6H2O.
      IR Raman spectra metal sulfate hydrate; copper sodium sulfate dihydrate
      vibrational spectra; transition metal methylammonium sulfate hexahydrate;
      zinc methylammonium disulfate hexahydrate vibrational spectra; nickel
      methylammonium disulfate hexahydrate vibrational spectra
      Hydrogen bond
          (intramol.; in transition metal methylammonium sulfate hexahydrates
          studied with vibrational spectra)
      IR spectra
      Molecular vibration
      Raman spectra
      Vibrational spectra
          (of copper sodium sulfate dihydrate and transition metal methylammonium sulfate hexahydrates)
      Transition metal salts
      RL: PEP (Physical, engineering or chemical process); PRP (Properties);
      PROC (Process)
          (vibrational spectra of copper, zinc, and nickel methylammonium sulfate
          hexahydrates)
      18901-72-9, Copper sodium sulfate (CuNa2(SO4)2) dihydrate Copper sodium sulfate (CuNa2(SO4)2) dideuterate
                                                                                      202406-41-5,
      RL: PEP (Physical, engineering or chemical process); PRP (Properties);
      PROC (Process)
          (IR and Raman spectra and internal vibrational mode assignments)
                        202406-47-1 202406-49-3
      202406-44-8
      RL: PEP (Physical, engineering or chemical process); PRP (Properties);
      PROC (Process)
          (IR and Raman spectra, internal vibrational mode assignments, and
          hydrogen bonding)
                  THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Abraham, S; J Raman Spectrosc 1991, V22, P245 CAPLUS
(2) Bachman, H; Naturwiss 1960, V47, P177
(3) Baran, J; J Mol Struct 1987, V162, P211 CAPLUS
(4) Bellanato, J; Spectrochim Acta 1960, V16, P1344 CAPLUS
(5) Campbell, J; Spectrochim Acta A 1970, V26, P2351 CAPLUS
(6) Dahlman, B; Ark Min 1952, V1, P230, CAPLUS
(6) Dahlman, B; Ark Min 1952, V1, P339 CAPLUS
(7) Fateley, W; Infrared and Raman Selection Rules for Molecular and Lattice Vibrations - The Correlation Method 1972
(8) Gattow, G; Act Crystallogr 1958, V11, P377 CAPLUS
(9) Gattow, G; Acta Crystallogr 1958, V11, P866 CAPLUS
(10) Gupta, S; J Mol Struct 1984, V112, P41 CAPLUS
(11) Herzberg, G; Infrared and Raman Spectra of Polyatomic Molecules 1966
(12) Hofmann, Z; Krist 1930, V75, P158
(13) Hofmann, Z; Krist 1931, V78, P279
(14) Ikawa, S; J Raman Spectrosc 1977, V6, P89 CAPLUS
(15) Jayakumar, V; Phys Status Solid 1988, V109, P635 CAPLUS
(16) Jordanovska, V; J Therm Anal 1992, V38, P1563 CAPLUS
(17) Kamoun, M; Spectrochim Acta A 1988, V44, P471
(18) Leone, M; Period Miner 1954, V23, P223 CAPLUS
 (19) Mathew, X; Ph D thesis, Chap 8, University of Kerala 1989
(20) Mazzi, F; Acta Crystallogr 1955, V8, P137 CAPLUS
```

```
(21) Montgomery, H; Acta Crystallogr 1966, V20, P659 CAPLUS (22) Montgomery, H; Acta Crystallogr 1966, V20, P728 CAPLUS (22) Montgomery, H; Acta Crystallogr 1966, V20, P728 CAPLUS
(23) Mylrajan, M; J Raman Spectrosc 1985, V16, P412 CAPLUS (24) Nakagawa, I; Spectrochim Acta A 1964, V20, P429 CAPLUS (25) Rajagopal, P; J Raman Spectrosc 1988, V19, P407
(25) Kajagopai, P; J Kaman Spectrosc 1988, V19, P407

(26) Rama Rao, V; Acta Crystallogr 1961, V14, P738

(27) Rao, C; Chemical Applications of Infrared Spectroscopy 1963

(28) Sekar, G; J Solid State Chem 1987, V66, P235 CAPLUS

(29) Sekar, G; J Solid State Chem 1988, V74, P424 CAPLUS

(30) Srinivasan, T; J Raman Spectrosc 1992, V23, P21 CAPLUS

(31) Srinivasan, T; Phase Transit 1992, V38, P97 CAPLUS

(32) Srivastava, J; J Phys C Solid State Phys 1988, V21, P4669 CAPLUS
           ANSWER 50 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
           184824-62-2 REGISTRY
RN
           Entered STN: 09 Jan 1997
ED
           Zinc, (1-butanamine) [methylphosphonato(2-)-κ0]- (9CI) (CA INDEX
CN
           NAME)
           C5 H14 N O3 P Zn
MF
           CCS
CI
           CA
SR
                                    CA, CAPLUS
           STN Files:
LC
              CAplus document type: Journal
               Roles from non-patents: PREP (Preparation); PRP (Properties)
```

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

#### REFERENCE 1

```
132:8432 CA
AN
       An organometallic route to zinc phosphonates and their intercalates
       Gerbier, Philippe; Guerin, Christian; Henner, Bernard; Unal, Jean-Remi U.M.R. 5637 -Universite Montpellier II, Montpellier, 34095, Fr. Journal of Materials Chemistry (1999), 9(10), 2559-2565
TI
ΑU
CS
SO
       CODEN: JMACEP; ISSN: 0959-9428
       Royal Society of Chemistry
PB
       Journal
DT
LA
       English
       78-3 (Inorganic Chemicals and Reactions)
CC
       An organometallic nonaq. route to zinc phosphonates and to their
AR
       intercalates was studied. Various phosphonic acids react with
       dimethylzinc in THF media to afford the corresponding layered zinc
       phosphonates Zn(03PR1) (R1 = Me, Ph, 2- and 3-thienyl, thiophen-3-ylmethyl) with evolution of methane. The presence of a primary n-alkylamine in the reaction mixture allows the 1-pot formation of
       2-dimensional-layered intercalated phases Zn(O3PR1) RNH2 [R2 = Bu, Penn (n-pentyl)] whereas a more bulky amine such as cyclohexylamine (HexcNH2) give 1-dimensional polymeric chains Zn(O3PPh) · 2HexcNH2.
       zinc phosphonate hydrate alkylamine intercalate prepn
ST
       Amines, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
IT
            (aliphatic, zinc intercalate complexes; preparation of zinc phosphonate
```

```
alkylamine intercalation compds. from organometallic nonaq. route,
          interlayer spacing and 31P CP MAS NMR spectra)
      NMR (nuclear magnetic resonance)
IT
           (phosphorus-31 CP MAS NMR spectra of zinc phosphonates and their
          hydrates and alkylamine intercalation compds., and relationship to
          phosphonate connectivity)
      Intercalation compounds
IT
      RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of zinc phosphonate alkylamine intercalation compds. from
          organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR
          spēctra)
      108-91-8, Cyclohexanamine, reactions 109-73-110-58-7, Pentylamine RL: RCT (Reactant); RACT (Reactant or reagent)
                                                          109-73-9, Butylamine, reactions
IT
          (for preparation of zinc phosphonate alkylamine intercalation compds. from
          organometallic nonaq. route)
                                                                                872-31-1,
                                               544-97-8, Dimethylzinc
      122-52-1, Triethylphosphite
IT
                               993-13-5, Methylphosphonic acid
                                                                             1003-09-4,
      3-Bromothiophene
                               1571-33-1, Phenylphosphonic acid
      2-Bromothiophene
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (for preparation of zinc phosphonates and their hydrates and alkylamine intercalation compds. from organometallic nonaq. route) 40-95-4P 21042-06-8P 113282-79-4P, 3-Thienylphosphonic acid
      13640-95-4P
IT
      113305-47-8P, 2-Thienylphosphonic acid 188565-0
Thiophen-3-ylmethylphosphonic acid 251323-56-5P
                                                             188565-05-1P,
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
           (for preparation of zinc phosphonates and their hydrates and alkylamine
           intercalation compds. from organometallic nonaq. route)
                                                                         115320-62-2P, Zinc
      72702-22-8P, Zinc phenylphosphonate monohydrate
IT
      methylphosphonate monohydrate 251323-48-5P, Zinc 2-thienylphosphonate monohydrate 251323-49-6P, Zinc 3-thienylphosphonate monohydrate 251323-50-9P, Zinc thiophen-3-ylmethylphosphonate monohydrate
      RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
           (preparation from organometallic nonaq. route, interlayer spacing and 31P CP
          MAS NMR spectrum)
                                                                  251323-51-0P
                                                                                      251323-52-1P
       162050-26-2P
                          162050-27-3P
                                               184824-62-2P
IT
                                               251323-55-4P
       251323-53-2P
                          251323-54-3P
      RL: PRP (Properties); SPN (Synthetic preparation); PREP_(Preparation)
           (preparation from organometallic nonaq. route, interlayer spacing and 31P CP
          MAS NMR spectrum of intercalate)
      133075-33-9P, Zinc methylphosphonate 251323-45-2P, Zinc 2-thienylphosphonate 251323-46-3P, Zinc 3-thienylphosphonate
                                                          251323-45-2P, Zinc
IT
                                                                                             251323-47
      -4P, Zinc thiophen-3-ylmethylphosphonate
      RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation from organometallic nonaq. route, interlayer spacing, 31P CP
           MAS NMR spectrum and hydration)
      34335-10-9P, Zinc phenylphosphonate
IT
      RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
           (preparation from organometallic nonaq. route, interlayer spacing, 31P CP
          MAS NMR spectrum, hydration and intercalation of alkylamines)
                  THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Alberti, G; Adv Mater 1996, V8, P291 CAPLUS
(2) Cao, G; Inorg Chem 1988, V27, P2781 CAPLUS
(3) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS
(4) Clearfield, A; Prog Inorg Chem 1998, P371 CAPLUS
(5) Corriu, R; J Mater Chem 1998, V8, P1827 CAPLUS
 6) Cunningham, D; Inorg Chim Acta 1979, V37, P95 CAPLUS
(7) Drumel, S; J Mater Chem 1996, V6, P1843 CAPLUS
```

```
(8) Ferey, G; C R Acad Sci Paris Ser IIc 1998, V1, P1 CAPLUS (9) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS (10) Hahn, F; Z Naturforsch Teil B 1990, V45, P134 CAPLUS
(11) Hix, G; J Mater Chem 1998, V8, P579 CAPLUS
(12) Iwao, M; Heterocycl Chem 1980, V17, P1259 CAPLUS
(13) Jones, A; Inorg Synth 1997, V31, P15 CAPLUS
(14) Judenstein, P; J Mater Chem 1996, V6, P511
(15) Keys, A; J Chem Soc Chem Commun 1995, P2339
(16) Kiss, T; Inorg Chim Acta 1987, V138, P25 CAPLUS
(17) Lugmair, C; Chem Mater 1997, V9, P339 CAPLUS
(18) Martin, K; Inorg Chim Acta 1989, V155, P7 CAPLUS
(19) Massiot, D; Chem Mater 1997, V9, P6 CAPLUS
(20) McKenna, C; Tetrahedron Lett 1977, P155 CAPLUS
(21) Montero, M; Angew Chem Int Ed Engl 1995, V34, P2504 CAPLUS
(22) Outlable L: Chem Mater 1997, V9, P1900 CAPLUS
(22) Ouahab, L; Chem Mater 1997, V9, P1909 CAPLUS (23) O'Hare, D; Inorganic Materials 2nd edn 1997, P172
(24) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS (25) Schubert, U; Chem Mater 1995, V7, P2010 CAPLUS (26) Scott, K; Chem Mater 1995, V7, P1095 CAPLUS (27) Tays, P; Chem Ber 1970, V103, P2428 CAPLUS
(28) Voigt, A; Angew Chem Int Ed Engl 1996, V35, P748 CAPLUS (29) Walawalkar, M; J Am Chem Soc 1997, V119, P4656 CAPLUS (30) Yang, Y; Angew Chem Int Ed 1999, V38, P664 CAPLUS (31) Yang, Y; J Chem Soc Dalton Trans 1996, P3609 CAPLUS (32) Zhang, Y; J Mater Chem 1995, V5, P315 CAPLUS
REFERENCE 2
         126:41873 CA
ΔN
        Structure of Zn(03PC2H4CO2H) 0.5C6H5NH2 and XANES-EXAFS study of
TI
         the intercalation of amines into Zn(O3PR)·H2O zinc
         alkylphosphonates
        Drumel, Stephanie; Janvier, Pascal; Bujoli-Doeuff, Martine; Bujoli, Bruno IMN, UMR CNRS 110, Faculte des Sciences et des Techniques, Nantes, 44072,
ΑU
CS
         Journal of Materials Chemistry (1996), 6(11), 1843-1847
SO
         CODEN: JMACEP; ISSN: 0959-9428
         Royal Society of Chemistry
PB
         Journal
DT
         English
LA
         78-7 (Inorganic Chemicals and Reactions)
CC
         Section cross-reference(s): 75
        From XANES-EXAFS expts., neither the dehydration nor the subsequent n-alkylamine intercalation in Zn(03PCH3) H20 appears to be
AB
         topotactic. On the contrary, the whole process consists of breaking Zn-O bonds present in the hydrated material, so that no bridging oxygen remains
         in the inorg. sheet. This hypothesis is supported by the structural
determination
         of an aniline intercalate: Zn(O3PC2H4CO2H)·0.5C6H5NH2
         [orthorhombic, space group Pbcn, a 29.880(6), b 8.526(2), c 14.720(3)
        Å, Z = 16, R = 0.043 and Rw = 0.047; 2063 observed reflections, I > 2\sigma(I)]. For steric reasons, only half of the zinc atoms are coordinated to aniline; the 2nd half of the metal atoms that are not bound to the amine retain the coordinate to the amine retain the coordinate.
         to the amine retain the environment present in the initial anhydrous phase. crystal structure zinc carboxyethylphosphonate aniline intercalated; zinc
ST
         carboxyethylphosphonate aniline intercalated prepn structure;
         alkylphosphonate zinc alkylamine intercalation
         EXAFS spectra
IT
         XANES spectra
               (of zinc alkylphosphonates and their aqua or butylamine intercalation
               complexes)
```

```
crystal structure
IT
     Molecular structure
         (of zinc carboxyethylphosphonate aniline intercalation complex) 075-33-9 166671-21-2 184824-61-1 184824-62-2
     133075-33-9
IT
     RL: PRP (Properties)
         (XANES-EXAFS spectra of)
     5962-42-5, 2-Carboxyethylphosphonic acid
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc carboxyethylphosphonate aniline intercalation complex)
     184824-60-0P
IT
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (polymeric; preparation and crystal structure of)
     ANSWER 51 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     182930-97-8 REGISTRY
RN
     Entered STN: 07 Nov 1996
ED
     Copper(2+), triaquabis(methanamine)(phosphine)-, (OC-6-22)- (9CI) (CA
CN
     INDEX NAME)
     C2 H19 Cu N2 O3 P
MF
     CCS
CI
SR
     CA
     STN Files:
                   CA, CAPLUS
LC
DT.CA CAplus document type: Journal
       Roles from non-patents: FORM (Formation, nonpreparative); PROC
        (Process); PRP (Properties); RACT (Reactant or reagent)
      NH2-Me
           OH<sub>2</sub>
           OH2
H20'
      NH2-Me
                 1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      125:286037 CA
AN
     Quantum-chemical studies on the mechanism of the novel reaction of
TI
     oxidative amination of P4 in the copper(II) coordination sphere
     Dorfman, Ya. A.; Abdreimova, R. R.
ΑU
     Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy
CS
      of Sciences of Kazakhstan, Almaty, Kazakhstan
     Russian Journal of Coordination Chemistry (Translation of
S<sub>0</sub>
     Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
CODEN: RJCCEY; ISSN: 1070-3284
     MAIK Nauka/Interperiodica
PR
DT
      Journal
      English
LA
     67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
     Section cross-reference(s): 65
     A novel fast and selective reaction of oxidative amination of P4 in the
AB
     toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant.
```

ST

IT

IT

IT

IT

IT

L9

RN

ED

CN

MF

CI SR

```
formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0)
                              The kinetics and mechanism of the novel reaction and
        at 20-80°C.
       the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed
        through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation
       of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to
        treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the
        d-character of Cu(II); to a considerable redox potential of the
       d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II)→Cu(O) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra-and interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions
        other ligands, thereby stimulating redox and acid-base reactions. mechanism oxidative amination phosphorus copper acidoamido; kinetics
        oxidative amination phosphorus copper acidoamido; quantum chem mechanism
        oxidative amination phosphorus
        Kinetics of amination
              (mechanism; quantum-chemical studies on mechanism of oxidative amination
             of P4 in copper(II) coordination sphere)
              (quantum-chemical studies on mechanism of oxidative amination of P4 in
              copper(II) coordination sphere)
        Molecular orbital
              (CNDO, quantum-chemical studies on mechanism of oxidative amination of P4
              in copper(II) coordination sphere)
                                                                                                           182930-81-0
                                                                                  182930-80-9
        182930-77-4
                                 182930-78-5
                                                         182930-79-6
                                                                                                          182930-86-5
182930-91-2
                                                                                  182930-85-4
                                 182930-83-2
                                                         182930-84-3
         182930-82-1
                                                         182930-89-8
                                                                                  182930-90-1
        182930-87-6
                                 182930-88-7
                                                                                                           182930-96-7
                                                                                  182930-95-6
                                 182930-93-4
                                                         182930-94-5
        182930-92-3
        RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (quantum-chemical studies on mechanism of oxidative amination of P4 in copper(II) coordination sphere)
        182930-97-8
        12185-10-3, Phosphorus(p4), reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
              (quantum-chemical studies on mechanism of oxidative amination of P4 in
              copper(II) coordination sphere)
        ANSWER 52 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
         182930-94-5 REGISTRY
         Entered STN: 07 Nov 1996
        Copper(1+), triaquachloro(methanamine)(phosphine)-, (OC-6-43)- (9CI)
         INDEX NAME)
         C H14 Cl Cu N 03 P
         CCS
        STN Files:
                               CA, CAPLUS
           CAplus document type: Journal
DT.CA
          Roles from non-patents: FORM (Formation, nonpreparative); PROC
```

(Process); PRP (Properties); RACT (Reactant or reagent)

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

125:286037 CA ΑN Quantum-chemical studies on the mechanism of the novel reaction of TI oxidative amination of P4 in the copper(II) coordination sphere

ΑU

Dorfman, Ya. A.; Abdreimova, R. R. Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy CS

of Sciences of Kazakhstan, Almaty, Kazakhstan

Russian Journal of Coordination Chemistry (Translation of S<sub>0</sub> Koordinatsionnaya Khimiya) (1996), 22(10), 716-729 CODEN: RJCCEY; ISSN: 1070-3284

MAIK Nauka/Interperiodica PB

Journal DT English LA

AB

67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) CC

section cross-reference(s): 65

A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHP)2 and P4(NHP)2. of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II)→Cu(O) transition in amino-pyridine solns.; and to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intraand interligand covalent and ionic interactions. As a result of the coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions. mechanism oxidative amination phosphorus copper acidoamido; kinetics

oxidative amination phosphorus copper acidoamido; quantum chem mechanism

oxidative amination phosphorus

ST

```
Kinetics of amination
IT
          (mechanism; quantum-chemical studies on mechanism of oxidative amination
         of P4 in copper(II) coordination sphere)
IT
          (quantum-chemical studies on mechanism of oxidative amination of P4 in
          copper(II) coordination sphere)
      Molecular orbital
IT
          (CNDO, quantum-chemical studies on mechanism of oxidative amination of P4
          in copper(II) coordination sphere)
                                                                            182930-81-0
                                         182930-79-6
                                                          182930-80-9
      182930-77-4
                       182930-78-5
IT
                                                                            182930-86-5
                                                          182930-85-4
                                         182930-84-3
      182930-82-1
                       182930-83-2
                                                                            182930-91-2
                                         182930-89-8
                       182930-88-7
                                                          182930-90-1
      182930-87-6
                                                          182930-95-6
                                                                            182930-96-7
                       182930-93-4
                                         182930-94-5
      182930-92-3
      182930-97-8
      RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (quantum-chemical studies on mechanism of oxidative amination of P4 in
          copper(II) coordination sphere)
      12185-10-3, Phosphorus(p4), reactions
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(quantum-chemical studies on mechanism of oxidative amination of P4 in
IT
          copper(II) coordination sphere)
      ANSWER 53 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      182930-88-7 REGISTRY
RN
      Entered STN: 07 Nov 1996
ED
      Cuprate(1-), trichlorobis(methanamine)(phosphine)-, (OC-6-21)- (9CI) (CA
CN
      INDEX NAME)
      C2 H13 C13 Cu N2 P
MF
      CCS
CI
SR
      CA
                      CA, CAPLUS
LC
      STN Files:
        CAplus document type: Journal
DT.CA
        Roles from non-patents: FORM (Formation, nonpreparative); PROC
         (Process): PRP (Properties); RACT (Reactant or reagent)
       NH2-Me
H<sub>3</sub>P
-c1
       NH2-Me
                   1 REFERENCES IN FILE CA (1907 TO DATE)
                   1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
AN
      Quantum-chemical studies on the mechanism of the novel reaction of
TI
      oxidative amination of P4 in the copper(II) coordination sphere
      Dorfman, Ya. A.; Abdreimova, R. R.
ΑU
      Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy
CS
```

```
of Sciences of Kazakhstan, Almaty, Kazakhstan
       Russian Journal of Coordination Chemistry (Translation of
SO
       Koordinatsionnaya Khimiya) (1996), 22(10), 716-729
        CODEN: RJCCEY; ISSN: 1070-3284
       MAIK Nauka/Interperiodica
PB
        Journal
DT
        English
LA
       67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
       Section cross-reference(s): 65
       A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant.
AB
       formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and
       the optimum conditions for its occurrence are studied by methods of 31P
       NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed
       through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of
        copper(II). The high rate of selectivity of the reaction is due to the
       d-character of Cu(II); to a considerable redox potential of the two-electron Cu(II) \rightarrow Cu(0) transition in amino-pyridine solns.; and
       to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intraand interligand covalent and ionic interactions. As a result of the
       coordination to metal, the reactants (P4 and amines) and the amide and triamidophosphite products become more polar and form strong bonds with other ligands, thereby stimulating redox and acid-base reactions.
        mechanism oxidative amination phosphorus copper acidoamido; kinetics
ST
        oxidative amination phosphorus copper acidoamido; quantum chem mechanism
        oxidative amination phosphorus
        Kinetics of amination
IT
             (mechanism; quantum-chemical studies on mechanism of oxidative amination
            of P4 in copper(II) coordination sphere)
        Amination
IT
             (quantum-chemical studies on mechanism of oxidative amination of P4 in
             copper(II) coordination sphere)
        Molecular orbital
IT
             (CNDO, quantum-chemical studies on mechanism of oxidative amination of P4
             in copper(II) coordination sphere)
930-77-4 182930-78-5 182930-79
                                                    182930-79-6
                                                                                                 182930-81-0
                                                                           182930-80-9
        182930-77-4
IT
                                                                          182930-85-4 182930-86-5
                                                    182930-84-3
                              182930-83-2
        182930-82-1
                                                                                                 182930-91-2
                                                                           182930-90-1
                              182930-88-7
                                                    182930-89-8
        182930-87-6
                                                                                                 182930-96-7
                                                                           182930-95-6
                                                    182930-94-5
        182930-92-3
                              182930-93-4
        182930-97-8
        RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
       process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (quantum-chemical studies on mechanism of oxidative amination of P4 in
             copper(II) coordination sphere)
        12185-10-3, Phosphorus(p4), reactions
IT
        RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
             (quantum-chemical studies on mechanism of oxidative amination of P4 in
             copper(II) coordination sphere)
```

```
ANSWER 54 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      182930-87-6 REGISTRY
RN
      Entered STN: 07 Nov 1996
ED
      Cuprate(2-), tetrachloro(methanamine)(phosphine)-, (OC-6-32)- (9CI) (CA
CN
      INDEX NAME)
      C H8 C14 Cu N P
MF
      CCS
CI
SR
      CA
                       CA, CAPLUS
      STN Files:
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PROC (Process); PRP (Properties); RACT (Reactant or reagent)
```

REFERENCE 1 AN 125:286037 CA Quantum-chemical studies on the mechanism of the novel reaction of oxidative amination of P4 in the copper(II) coordination sphere TI Dorfman, Ya. A.; Abdreimova, R. R. ΑU Sokol'skii Institute of Organic Caltalysis and Electrochemistry, Academy CS of Sciences of Kazakhstan, Almaty, Kazakhstan Russian Journal of Coordination Chemistry (Translation of S<sub>0</sub> Koordinatsionnaya Khimiya) (1996), 22(10), 716-729 CODEN: RJCCEY; ISSN: 1070-3284 MAIK Nauka/Interperiodica PB Journal DT English LA 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) CC Section cross-reference(s): 65 A novel fast and selective reaction of oxidative amination of P4 in the toluene-pyridine solns. of Cu(II) acidoamido complexes results in a quant. AB formation of triamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR and Cu(0) at 20-80°C. The kinetics and mechanism of the novel reaction and the optimum conditions for its occurrence are studied by methods of 31P NMR, IR, and UV spectroscopy, gas chromatog., kinetics, redox potentiometry, thermodn., chemical modeling, orbital symmetry, and the quantum-chemical method of the CNDO. The reaction is found to proceed through the two principal steps: oxidative amination of P4 to triamidophosphites (RHN)3P and (R2N)3P through the intermediate formation of diamidotetraphosphines P4(NHR)2 and P4(NR2)2, tetraamidotetraphosphines P4(NHR)4 and P4(NR2)4, and tetraamidodiphosphines P2(NHR)4 and P2(NR2)4, followed by the oxidative imination of triamidophosphites to treamidophosphazoalkanes (RHN)3P=NR and (R2N)3P=NR in the inner sphere of copper(II). The high rate of selectivity of the reaction is due to the d-character of Cu(II); to a considerable redox potential of the

```
two-electron Cu(II)→Cu(O) transition in amino-pyridine solns.; and
     to the advantageous charge delocalization in P4, in its intermediate oxidation products, in amines RH2N and R2HN, in amides RHN- and R2N-, and in triamidophosphites (RHN)3P and (R2N)3P, favoring the changes in the intra-
     and interligand covalent and ionic interactions. As a result of the
     coordination to metal, the reactants (P4 and amines) and the amide and
     triamidophosphite products become more polar and form strong bonds with
     other ligands, thereby stimulating redox and acid-base reactions.
     mechanism oxidative amination phosphorus copper acidoamido; kinetics
ST
     oxidative amination phosphorus copper acidoamido; quantum chem mechanism
     oxidative amination phosphorus
     Kinetics of amination
IT
         (mechanism; quantum-chemical studies on mechanism of oxidative amination
         of P4 in copper(II) coordination sphere)
IT
     Amination
         (quantum-chemical studies on mechanism of oxidative amination of P4 in
         copper(II) coordination sphere)
     Molecular orbital
         (CNDO, quantum-chemical studies on mechanism of oxidative amination of P4
IT
         in copper(II) coordination sphere)
                                                                    182930-81-0
                                                     182930-80-9
                                     182930-79-6
     182930-77-4
                     182930-78-5
IT
                                                                    182930-86-5
                                     182930-84-3
                                                     182930-85-4
                     182930-83-2
     182930-82-1
                                                                    182930-91-2
                                     182930-89-8
                                                     182930-90-1
                     182930-88-7
     182930-87-6
                                                                    182930-96-7
                                                     182930-95-6
                     182930-93-4
                                     182930-94-5
     182930-92-3
     182930-97-8
     RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
     process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
         (quantum-chemical studies on mechanism of oxidative amination of P4 in
         copper(II) coordination sphere)
      12185-10-3, Phosphorus(p4), reactions
IT
     RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
      (Reactant); PROC (Process); RACT (Reactant or reagent)
         (quantum-chemical studies on mechanism of oxidative amination of P4 in
         copper(II) coordination sphere)
      ANSWER 55 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      173178-23-9 REGISTRY
Entered STN: 13 Feb 1996
RN
ED
     Cobalt, pentakis(methanamine)[phosphato(3-)-0]-, (OC-6-22)- (9CI)
CN
      INDEX NAME)
      C5 H25 Co N5 O4 P
MF
      CCS, COM
CI
SR
      CA
      STN Files:
                    CA, CAPLUS
LC
        CAplus document type:
                                 Journal
DT.CA
        Roles from non-patents: PROC (Process); PRP (Properties); RACT
RL.NP
        (Reactant or reagent)
              NH2-Me
 Me-NH2
```

```
124:128031 CA
AN
         Outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
TI
          complexes. A temperature- and pressure-dependence kinetic study on the effects of the different {N5} groups
          Martinez, Manuel; Pitarque, Mari-Angel
ΑU
          Facultat Quimica, Universitat Barcelona, Barcelona, E-08028, Spain Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry
CS
S0
          (1995), (24), 4107-11
CODEN: JCDTBI; ISSN: 0300-9246
          Royal Society of Chemistry
PB
          Journal
DT
          English
LA
          67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 69, 78
CC
          Outer-sphere redox reactions between [Co\{N5\}(HnPO4)]n+[\{N5\} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane (L)] and <math>[Fe(CN)6]4- have been studied as a function of pH, \{N5\}, temperature and
AB
          pressure. The effect of the size of the \{N5\} skeleton, has been investigated for the n = 0, 1, 2 systems in order to establish possible correlations between the size and charge of the cobalt(III) complex and
          the ion-pair formation constant, the electron-transfer rate constant, and the
          thermal and baric activation parameters. The values obtained indicate that the ion-pair formation consts. are the same, within exptl. error, for
           all the systems studied. The electron-transfer rate constant for a given
          degree (n = 1) of protonation of the [Co{N5}(HnPO4)]n+ complex increases on increasing the size of the monodentate amines, while an important decrease is observed when they are substituted by the N5 macrocycle (L) [2.6]
          + 10-3 s-1, \{N5\} = (NH3)5, 59 + 10-3 s-1, \{N5\} = (NH2Me)5, 0.73 + 10-3 s-1, \{N5\} = L; resp. at 35°C]. The activation enthalpies do not show any significant change, neither with decreasing charge on the cobalt complex nor with the size of the amine. The values of \Delta S. thermod. and \Delta V. thermod. vary considerably with the
          degree of protonation of the phosphate ligands and the size of the CoIII cavity of the complexes. The opposite trends observed for the values of \Delta s. thermod. [8 J K-1 mol-1 for {N5} = (NH2Me)5 (n = 1); -61 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 32 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 17 cm3 mol-1 for {N5} = (NH3)5 (n = 0)] are related to the existence of an important increase in hydrogen bond formation in the cobalt(III) complex
           on going to the transition state.
           cobalt macrocycle complex redox reaction kinetics
           Electron exchange and Charge transfer
           Protonation and Proton transfer reaction
           Redox reaction
                 (outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
                 complexes)
           Hydrogen bond
 IT
           Ion pairs
           Kinetics of electron exchange
Kinetics of protonation
Kinetics of redox reaction
                 (outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
                 complexes and temperature- and pressure-dependence kinetic effects of
                 different {N5})
```

```
19306-79-7
                                                                                     173178-22-8
                                              19169-72-3
                          15612-03-0
       13408-63-4
IT
       173178-23-9
                          173178-24-0
       RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
            complexes and temperature- and pressure-dependence kinetic effects of
            different {N5})
       ANSWER 56 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN 173178-22-8 REGISTRY Entered STN: 13 Feb 1996
L9
RN
ED
       Cobalt, pentakis(methanamine)[phosphato(3-)-0]-, conjugate monoacid,
CN
       (OC-6-22)- (9CI) (CA INDEX NAME)
C5 H25 CO N5 O4 P . H
MF
CI
       CCS
SR
                        CA, CAPLUS
       STN Files:
LC
          CAplus document type: Journal Roles from non-patents: PROC (Process); PRP (Properties); RACT
DT.CA
           (Reactant or reagent)
       (173178-23-9)
CRN
                   NH2-Me
             NH2-Me
```

● H<sup>+</sup>

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

124:128031 CA Outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, TT (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane] complexes. A temperature- and pressure-dependence kinetic study on the effects of the different {N5} groups Martinez, Manuel; Pitarque, Mari-Angel Facultat Quimica, Universitat Barcelona, Barcelona, E-08028, Spain ΑU CS Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry SO (1995), (24), 4107-11 CODEN: JCDTBI; ISSN: 0300-9246 Royal Society of Chemistry PB Journal DT English LA 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) CC Section cross-reference(s): 69, 78

```
Outer-sphere redox reactions between [Co{N5}(HnPO4)]n+[{N5}] = (NH3)5
AB
        (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane (L)] and
        [Fe(CN)6]4- have been studied as a function of pH, {N5}, temperature and pressure. The effect of the size of the {N5} skeleton, has been
        investigated for the n=0,\ 1,\ 2 systems in order to establish possible correlations between the size and charge of the cobalt(III) complex and
        the ion-pair formation constant, the electron-transfer rate constant, and the
        thermal and baric activation parameters. The values obtained indicate that the ion-pair formation consts. are the same, within exptl. error, for
        all the systems studied. The electron-transfer rate constant for a given
        degree (n = 1) of protonation of the [Co\{N5\}(HnPO4)]n+ complex increases on increasing the size of the monodentate amines, while an important
        decrease is observed when they are substituted by the N5 macrocycle (L) [2.6
       + 10-3 s-1, {N5} = (NH3)5, 59 + 10-3 s-1, {N5} = (NH2Me)5, 0.73 + 10-3 s-1, {N5} = L; resp. at 35°C]. The activation enthalpies do not show any significant change, neither with decreasing
        charge on the cobalt complex nor with the size of the amine. The values
       cnarge on the cobait complex nor with the size of the amine. The values of \Delta S. thermod. and \Delta V. thermod. vary considerably with the degree of protonation of the phosphate ligands and the size of the CoIII cavity of the complexes. The opposite trends observed for the values of \Delta S. thermod. [8 J K-1 mol-1 for {N5} = (NH2Me)5 (n = 1); -61 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 32 J K-1 mol-1 for {N5} = (NH3)5 (n = 1); 17 cm3 mol-1 for {N5} = (NH3)5 (n = 0)] are related to the existence of an important increase in hydrogen bond formation in the cobalt(III) complex on going to the transition state
        on going to the transition state.
        cobalt macrocycle complex redox reaction kinetics
        Electron exchange and Charge transfer
IT
        Protonation and Proton transfer reaction
        Redox reaction
             (outer-sphere redox reactions of [COIII(N5)(HnPO4)]n+ [{N5} = (NH3)5,
             (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
             complexes)
        Hydrogen bond
IT
        Ion pāirs
        Kinetics of electron exchange
Kinetics of protonation
Kinetics of redox reaction
             (outer-sphere redox reactions of [CoIII{N5}(HnPO4)]n+ [{N5} = (NH3)5,
             (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
             complexes and temperature- and pressure-dependence kinetic effects of
             different {N5})
                                                 19169-72-3
                                                                      19306-79-7
                                                                                           173178-22-8
                             15612-03-0
IT
        13408-63-4
                              173178-24-0
        173178-23-9
        RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (outer-sphere redox reactions of [COIII{N5}(HnPO4)]n+ [{N5} = (NH3)5, (NH2Me)5 or 10-amino-10-methyl-1,4,8,12-tetraazacyclopentadecane]
             complexes and temperature- and pressure-dependence kinetic effects of
             different {N5})
        ANSWER 57 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        162050-26-2 REGISTRY
RN
        Entered STN: 07 Apr 1995
ED
        Zinc, (1-butanamine)[pheny]phosphonato(2-)-\kappa0]-(9CI)
                                                                                               (CA INDEX
CN
        NAME)
OTHER CA INDEX NAMES:
        Zinc, (1-butanamine)[phenylphosphonato(2-)-0]-
        C10 H16 N O3 P Zn
MF
        CCS
CI
SR
        STN Files: CA, CAPLUS
LC
```

DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

Ring System Data

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
========= C6	+=======   C6	-====================================	C6	46.150.18	1

3 REFERENCES IN FILE CA (1907 TO DATE) 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

132:8432 CA AN An organometallic route to zinc phosphonates and their intercalates Gerbier, Philippe; Guerin, Christian; Henner, Bernard; Unal, Jean-Remi U.M.R. 5637 -Universite Montpellier II, Montpellier, 34095, Fr. Journal of Materials Chemistry (1999), 9(10), 2559-2565 CODEN: JMACEP; ISSN: 0959-9428 TI ΑU CS 50 Royal Society of Chemistry PB Journal DT English LA 78-3 (Inorganic Chemicals and Reactions) CC An organometallic nonaq. route to zinc phosphonates and to their intercalates was studied. Various phosphonic acids react with AB dimethylzinc in THF media to afford the corresponding layered zinc dimethylzinc in THF media to afford the corresponding layered zinc phosphonates Zn(O3PR1) (R1 = Me, Ph, 2- and 3-thienyl, thiophen-3-ylmethyl) with evolution of methane. The presence of a primary n-alkylamine in the reaction mixture allows the 1-pot formation of 2-dimensional-layered intercalated phases Zn(O3PR1)·RNH2 [R2 = Bu, Penn (n-pentyl)] whereas a more bulky amine such as cyclohexylamine (HexcNH2) give 1-dimensional polymeric chains Zn(O3PPh)·2HexcNH2. zinc phosphonate hydrate alkylamine intercalate prepn ST Amines, preparation
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(aliphatic, zinc intercalate complexes; preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route, IT interlayer spacing and 31P CP MAS NMR spectra) NMR (nuclear magnetic resonance) IT (phosphorus-31 CP MAS NMR spectra of zinc phosphonates and their hydrates and alkylamine intercalation compds., and relationship to phosphonate connectivity) Intercalation compounds IT RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation of zinc phosphonate alkylamine intercalation compds. from organometallic nonaq. route, interlayer spacing and 31P CP MAS NMR

108-91-8, Cyclohexanamine, reactions 109-73-9, Butylamine, reactions 110-58-7, Pentylamine

IT

spectra)

```
RL: RCT (Reactant); RACT (Reactant or reagent)
              (for preparation of zinc phosphonate alkylamine intercalation compds. from
              organometallic nonaq. route)
                                                            544-97-8, Dimethylzinc
                                                                                                       872-31-1,
        122-52-1, Triethylphosphite
IT
                                         993-13-5, Methylphosphonic acid
                                                                                                    1003-09-4,
        3-Bromothiophene
                                         1571-33-1, Phenylphosphonic acid
        2-Bromothiophene
        RL: RCT (Reactant); RACT (Reactant or reagent)
              (for preparation of zinc phosphonates and their hydrates and alkylamine
              intercalation compds. from organometallic nonaq. route)
40-95-4P 21042-06-8P 113282-79-4P, 3-Thienylphosphonic acid
        13640-95-4P
IT
        113305-47-8P, 2-Thienylphosphonic acid 188565-05-1P, Thiophen-3-ylmethylphosphonic acid 251323-56-5P
        RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
         (Reactant or reagent)
              (for preparation of zinc phosphonates and their hydrates and alkylamine
              intercalation compds. from organometallic nonaq. route)
                                                                                               115320-62-2P, Zinc
        72702-22-8P, Zinc phenylphosphonate monohydrate
IT
                                                              251323-48-5P, Zinc 2-thienylphosphonate
        methylphosphonate monohydrate
        monohydrate 251323-49-6P, Zinc 3-thienylphosphonate monohydrate 251323-50-9P, Zinc thiophen-3-ylmethylphosphonate monohydrate
        RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation from organometallic nonaq. route, interlayer spacing and 31P CP
              MAS NMR spectrum)
                                                                                      251323-51-0P
                                                                                                                251323-52-1P
                                                            184824-62-2P
         162050-26-2P
                                  162050-27-3P
IT
                                                             251323-55-4P
                                  251323-54-3P
         251323-53-2P
         RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
               (preparation from organometallic nonaq. route, interlayer spacing and 31P CP
              MAS NMR spectrum of intercalate)
                                                                            251323-45-2P, Zinc
         133075-33-9P, Zinc methylphosphonate
IT
                                                251323-46-3P, zinc 3-thienylphosphonate
                                                                                                                         251323-47
         2-thienvlphosphonate
        -4P, Zinc thiophen-3-ylmethylphosphonate
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
    (preparation from organometallic nonaq. route, interlayer spacing, 31P CP
    MAS NMR spectrum and hydration)
34335-10-9P, Zinc phenylphosphonate
IT
         RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
         (Preparation); RACT (Reactant or reagent)
              (preparation from organometallic nonaq. route, interlayer spacing, 31P CP
              MAS NMR spectrum, hydration and intercalation of alkylamines)
                        THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THI

(1) Alberti, G; Adv Mater 1996, V8, P291 CAPLUS

(2) Cao, G; Inorg Chem 1988, V27, P2781 CAPLUS

(3) Cao, G; Inorg Chem 1991, V30, P1434 CAPLUS

(4) Clearfield, A; Prog Inorg Chem 1998, P371 CAPLUS

(5) Corriu, R; J Mater Chem 1998, V8, P1827 CAPLUS

(6) Cunningham, D; Inorg Chim Acta 1979, V37, P95 CAPLUS

(7) Drumel, S; J Mater Chem 1996, V6, P1843 CAPLUS

(8) Ferey, G; C R Acad Sci Paris Ser IIc 1998, V1, P1 CAPLUS

(9) Frink, K; Inorg Chem 1991, V30, P1438 CAPLUS

(10) Hahn, F; Z Naturforsch Teil B 1990, V45, P134 CAPLUS

(11) Hix. G: J Mater Chem 1998, V8, P579 CAPLUS
RE.CNT
(11) Hix, G; J Mater Chem 1998, V8, P579 CAPLUS
(12) Iwao, M; Heterocycl Chem 1980, V17, P1259 CAPLUS
(13) Jones, A; Inorg Synth 1997, V31, P15 CAPLUS
(14) Judenstein, P; J Mater Chem 1996, V6, P511
(15) Keys, A; J Chem Soc Chem Commun 1995, P2339
(16) Kiss, T: Thora Chim Acta 1987, V138, P25 CAPLUS
(16) Kiss, T; Inorg Chim Acta 1987, V138, P25 CAPLUS (17) Lugmair, C; Chem Mater 1997, V9, P339 CAPLUS (18) Martin, K; Inorg Chim Acta 1989, V155, P7 CAPLUS (19) Massiot, D; Chem Mater 1997, V9, P6 CAPLUS (20) McKenna, C; Tetrahedron Lett 1977, P155 CAPLUS
```

- (21) Montero, M; Angew Chem Int Ed Engl 1995, V34, P2504 CAPLUS (22) Ouahab, L; Chem Mater 1997, V9, P1909 CAPLUS (23) O'Hare, D; Inorganic Materials 2nd edn 1997, P172 (23) U Hare, D; Inorganic Materials 2nd edn 1997, P172 (24) Poojary, D; J Am Chem Soc 1995, V117, P11278 CAPLUS (25) Schubert, U; Chem Mater 1995, V7, P2010 CAPLUS (26) Scott, K; Chem Mater 1995, V7, P1095 CAPLUS (27) Tavs, P; Chem Ber 1970, V103, P2428 CAPLUS (28) Voigt, A; Angew Chem Int Ed Engl 1996, V35, P748 CAPLUS (29) Walawalkar, M; J Am Chem Soc 1997, V119, P4656 CAPLUS (30) Vang V: Angew Chem Int Ed 1999 (30) Yang, Y; Angew Chem Int Ed 1999, V38, P664 CAPLUS (31) Yang, Y; J Chem Soc Dalton Trans. 1996, P3609 CAPLUS. (32) Zhang, Y; J Mater Chem 1995, V5, P315 CAPLUS REFERENCE 2 124:67877 CA ΑN Coordinative intercalation of alkylamines into layered zinc TI phenylphosphonate. Crystal structures from x-ray powder diffraction data Poojary, Damodara M.; Clearfield, Abraham ΑU Department of Chemistry, Texas AM University, College Station, TX, 77843, Journal of the American Chemical Society (1995), 117(45), 11278-84 S0 CODEN: JACSAT; ISSN: 0002-7863 American Chemical Society PB Journal DT English 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) CC Section cross-reference(s): 75, 78 Zn phenylphosphonate monohydrate takes up 1 mol of amine when contacted with liquid primary alkylamines. The mechanism of intercalation involves replacement of the coordinated H20 mol. by the amine mols. Although the composition of the intercalate Zn(03PPh) (RNH2) is consistent with the anal. and spectroscopic data, there exist discrepancies in the observed interlayer d spacings of the intercalate with respect to that in the host compound The d spacing for the propylamine intercalate is in fact smaller than that in Zn phenylphosphonate itself. To understand this feature specifically and to explain the mechanism of amine intercalation in metal phosphonates in general, the authors determined the structures of the intercalates. The structures of Zn(03PPh)(RNH2), R = -C3H9 (1), -C4H11 (2), -C5H13 (3), were solved ab initio from x-ray powder diffraction data and refined by Rietveld methods. All the compds. are isostructural, and they crystallize in the monoclinic space group P21/c with a 13.978(3), b 8.791(2), c 9.691(2) Å, and  $\beta$  102.08(1)° for 1, a 14.698(4), b 8.957(3), c 9.712(3) Å, and  $\beta$  102.465(3)° for 2, and a 16.267(3), b 8.935(2), c 9.695(2) Å, and  $\beta$  102.32(1)° for 3. The structures of these intercalates are new and are different from that of the host compound although all of them are layered. In the In phenylphosphonate monohydrate takes up 1 mol of amine when contacted AΒ that of the host compound although all of them are layered. In the intercalate the Zn atoms are tetrahedrally coordinated as opposed to octahedral coordination in the host compound coordinative intercalation alkylamine zinc phenylphosphonate structure; intercalation coordinative alkylamine zinc phenylphosphonate structure ST Inclusion reaction IT (intercalation, of zinc phenylphosphonate monohydrate by alkylamines) 107-10-8, Propylamine, reactions 109-73-9, Butylamine, reactions IT
- IT 10/-10-8, Propylamine, reactions 109-/3-9, Butylamine, reactions
  110-58-7, Pentylamine 72702-22-8
  RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
  (coordinative intercalation of alkylamines into layered zinc
  phenylphosphonate and crystal structures from x-ray powder diffraction
  data)
- IT 162050-25-1P 162050-26-2P 162050-27-3P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

REFERENCE 3

# (preparation and crystal structure of)

```
122:229146 CA
AN
       Intercalation of alkylamines into dehydrated and hydrated zinc
TI
       phenylphosphonates
       Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
Department of Chemistry, Texas A and M Univ., College Station, TX, 77843,
ΑU
CS
       Journal of Materials Chemistry (1995), 5(2), 315-18
SO
       CODEN: JMACEP; ISSN: 0959-9428
       Royal Society of Chemistry
PB
       Journal
DT
       English
LA
       78-3 (Inorganic Chemicals and Reactions)
CC
       Primary amines, CnH2n+1NH2 (n = 3-8), were intercalated into layered anhydrous Zn phenylphosphonate Zn(O3PPh) and its monohydrate Zn(O3PPh). H2O
AB
       when the host compds. were brought into contact with liquid amines. In both cases, 1 mol of amine was intercalated forming layered compds. Zn(O3PPh).(RNH2) as characterized by powder x-ray diffraction, TG and IR
       spectroscopy. The amines coordinate to the Zn atoms at the site vacated by the H2O mol. A plot of the interlayer distances of the intercalates vs. the number of C atoms in the alkyl chain of the amine gives a straight line with a slope of 1.24 Å, which indicates that the alkyl chains are
       most likely packed as an interdigitated monolayer with a tilt angle of 78° with respect to the mean plane of the layer. A comparison of the intercalation reactions of Zn, Co and Cu Me- and phenyl-phosphonates is included in the discussion section.
       intercalation alkylamine dehydrated hydrated zinc phenylphosphonate; amine
ST
        alkyl intercalation zinc phenylphosphonate
       Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
  (intercalation of dehydrated and hydrated zinc phenylphosphonates by)
IT
        Molecular orientation
IT
             (of amines in amine intercalated zinc phenylphosphonates)
        Inclusion reaction
IT
             (intercalation, of alkylamines with dehydrated and hydrated zinc
             phenylphosphonates)
        34335-10-9, Phosphonic acid, phenyl-, zinc salt (1:1) RL: RCT (Reactant); RACT (Reactant or reagent)
                                                                                              72702-22-8
IT
             (intercalation reaction with alkylamines)
                                            nine 107-10-8, Propylamine, reactions
110-58-7, Pentylamine 111-26-2, Hexyl
111-86-4, Octylamine 112-20-9, Nonyla
                                                                                                            109-73-9.
        96-15-1, 2-Methylbutylamine
IT
                                                                                 111-26-2, Hexylamine
        Butylamine, reactions
                                                                                112-20-9, Nonylamine
        111-68-2, Heptylamine 111-86-4, Octylamine 123-82-0, 2-Aminoheptane RL: RCT (Reactant); RACT (Reactant or reagent)
             (intercalation reaction with dehydrated and hydrated phenylphosphonate)
        162050-25-1P
IT
                                                      162050-32-0P
                                                                             162050-33-1P
                               162050-31-9P
        162050-30-8P
        RL: SPN (Synthetic preparation); PREP (Preparation)
             (preparation of)
        ANSWER 58 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        162050-25-1 REGISTRY
Entered STN: 07 Apr 1995
RN
ΕD
        Zinc, [phenylphosphonato(2-)-0](1-propanamine)- (9CI) (CA INDEX NAME)
CN
        C9 H14 N 03 P Zn
MF
        CCS
CI
SR
        CA
        STN Files:
                           CA, CAPLUS
LC
```

DT.CA CAplus document type: Journal Roles from non-patents: PREP (Preparation); PRP (Properties)

Ring System Data

Elemental	Elemental	Size of	Ring System	Taentitier	RID
Analysis	Sequence	the Rings	Formula		Occurrence
EA	ES	SZ	RF		Count
======================================	+======   C6	+=======-   6	C6	46.150.18	1

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

124:67877 CA AN Coordinative intercalation of alkylamines into layered zinc TI phenylphosphonate. Crystal structures from x-ray powder diffraction data Poojary, Damodara M.; Clearfield, Abraham ΑU Department of Chemistry, Texas AM University, College Station, TX, 77843, CS Journal of the American Chemical Society (1995), 117(45), 11278-84 **S0** CODEN: JACSAT; ISSN: 0002-7863 American Chemical Society PB

Journal DT English LA

67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) CC

Section cross-reference(s): 75, 78

Zn phenylphosphonate monohydrate takes up 1 mol of amine when contacted with liquid primary alkylamines. The mechanism of intercalation involves replacement of the coordinated H20 mol. by the amine mols. Although the composition of the intercalate Zn(O3PPh)(RNH2) is consistent with the anal. and spectroscopic data, there exist discrepancies in the observed interlayer d spacings of the intercalate with respect to that in the host compound The d spacing for the propylamine intercalate is in fact smaller than that in Zn phenylphosphonate itself. To understand this feature specifically and to explain the mechanism of amine intercalation in metal phosphonates in general, the authors determined the structures of the intercalates. The structures of Zn(O3PPh)(RNH2), R = -C3H9 (1), -C4H11 (2), -C5H13 (3), were solved ab initio from x-ray powder diffraction data and refined by Rietveld methods. All the compds. are isostructural, and they crystallize Section cross-reference(s): 75, 78 AB Rietveld methods. All the compds. are isostructural, and they crystallize Rietveld methods. All the compds. are isostructural, and they crystalling the monoclinic space group P21/c with a 13.978(3), b 8.791(2), c 9.691(2) Å, and  $\beta$  102.08(1)° for 1, a 14.698(4), b 8.957(3), c 9.712(3) Å, and  $\beta$  102.465(3)° for 2, and a 16.267(3), b 8.935(2), c 9.695(2) Å, and  $\beta$  102.32(1)° for 3. The structures of these intercalates are new and are different from that of the host compound although all of them are layered. In the intercalate the Zn atoms are tetrahedrally coordinated as opposed to octahedral coordination in the host compound coordinative intercalation alkylamine zinc phenylphosphonate structure; intercalation coordinative alkylamine zinc phenylphosphonate structure ST

intercalation coordinative alkylamine zinc phenylphosphonate structure

```
Inclusion reaction
IT
                   (intercalation, of zinc phenylphosphonate monohydrate by alkylamines)
                                                                                             109-73-9, Butylamine, reactions
           107-10-8, Propylamine, reactions
IT
           110-58-7, Pentylamine 72702-22-8
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
  (coordinative intercalation of alkylamines into layered zinc phenylphosphonate and crystal structures from x-ray powder diffraction
                  data)
                                                                                  162050-27-3P
           162050-25-1P
                                              162050-26-2P
IT
           RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
                   (preparation and crystal structure of)
REFERENCE 2
            122:229146 CA
           Intercalation of alkylamines into dehydrated and hydrated zinc
TI
           phenylphosphonates
           Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
Department of Chemistry, Texas A and M Univ., College Station, TX, 77843,
ΑU
CS
            USA
            Journal of Materials Chemistry (1995), 5(2), 315-18
SO
           CODEN: JMACEP; ISSN: 0959-9428
Royal society of Chemistry
PB
            Journal
DT
            English
LA
            78-3 (Inorganic Chemicals and Reactions)
CC
            Primary amines, CnH2n+1NH2 (n = 3-8), were intercalated into layered
AΒ
            anhydrous Zn phenylphosphonate Zn(O3PPh) and its monohydrate Zn(O3PPh).H2O
           annygrous Zn pnenyipnospnonate Zn(O3PPn) and its mononygrate Zn(O3PPn).H20 when the host compds. were brought into contact with liquid amines. In both cases, 1 mol of amine was intercalated forming layered compds. Zn(O3PPh).(RNH2) as characterized by powder x-ray diffraction, TG and IR spectroscopy. The amines coordinate to the Zn atoms at the site vacated by the H20 mol. A plot of the interlayer distances of the intercalates vs. the number of C atoms in the alkyl chain of the amine gives a straight line with a slope of 1.24 Å, which indicates that the alkyl chains are most likely marked as an interdigitated monolayer with a tilt angle of
            most likely packed as an interdigitated monolayer with a tilt angle of
            78° with respect to the mean plane of the layer. A comparison of the intercalation reactions of Zn, Co and Cu Me- and phenyl-phosphonates
            is included in the discussion section.
            intercalation_alkylamine dehydrated hydrated zinc phenylphosphonate; amine
ST
            alkyl intercalation zinc phenylphosphonate
            Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
IT
                    (intercalation of dehydrated and hydrated zinc phenylphosphonates by)
            Molecular orientation
IT
                    of amines in amine intercalated zinc phenylphosphonates)
            Inclusion reaction
IT
                    (intercalation, of alkylamines with dehydrated and hydrated zinc
                   phenylphosphonates)
             34335-10-9, Phosphonic acid, phenyl-, zinc salt (1:1)
                                                                                                                                                72702-22-8
IT
            RL: RCT (Reactant); RACT (Reactant or reagent)
                    (intercalation reaction with alkylamines)
            96-15-1, 2-Methylbutylamine 107-10-8, Propylamine, reactions Butylamine, reactions 110-58-7, Pentylamine 111-26-2, Hexyl 111-68-2, Heptylamine 111-86-4, Octylamine 112-20-9, Nonylamine 112-20-9, Non
IT
                                                                                                                           111-26-2, Hexylamine
            111-68-2, Heptylamine
                                                                                                                           112-20-9, Nonylamine
             123-82-0, 2-Aminoheptane
             RL: RCT (Reactant); RACT (Reactant or reagent)
                    (intercalation reaction with dehydrated and hydrated phenylphosphonate)
                                                                                                                       162050-28-4P
                                                                                                                                                          162050-29-5P
                                               162050-26-2P
                                                                                   162050-27-3P
             162050-25-1P
IT
                                                                                   162050-32-0P
                                                                                                                       162050-33-1P
                                               162050-31-9P
             162050-30-8P
             RL: SPN (Synthetic preparation); PREP (Preparation)
```

# (preparation of)

```
ANSWER 59 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     147578-80-1 REGISTRY
RN
     Entered STN: 14 May 1993
     Copper, bis(1-butanamine)[phenylphosphonato-0]- (9CI) (CA INDEX NAME) C14 H27 Cu N2 O3 P
ED
CN
MF
     CCS
CI
SR
     CA
     STN Files:
                 CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
```

# Ring System Data

	Elemental	Size of	Ring System	Ring	RID
	Sequence	the Rings	Formula	Identifier	Occurrence
	ES	SZ	RF	RID	Count
======================================	+======-   c6	+== <b>===</b> ===-   6	C6	46.150.18	1

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
118:234154 CA
AN
             Intercalation of alkylamines into layered copper phosphonates
TI
             Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
ΑU
            Dep. Chem., Texas A and M Univ., College Station, Tx, 77843, USA Chemistry of Materials (1993), 5(4), 495-9
CS
50
             CODEN: CMATEX; ISSN: 0897-4756
DT
             Journal
             English
LA
             29-7 (Organometallic and Organometalloidal Compounds)
CC
            Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate.
AΒ
            of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PCH5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3) (RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates intercalation alkylamine layered dehydrated copper phosphonate; inclusion reaction alkylamine layered copper phosphonate
ST
             Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
IT
                     (alkyl, intercalation of, into layered copper phosphonates)
```

```
Inclusion reaction
IT
        (intercalation, of alkylamines into layered copper phosphonates)
     107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 1
IT
     109-73-9P, Butylamine, preparation
                   111-68-2P, 1-Heptanamine 111-86-4P, Octylamine
     Hexylamine
     RL: PREP (Preparation)
         (intercalation of, into layered copper phosphonates)
86-30-9 71803-57-1 147578-73-2
     45986-30-9
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (interlayer spacing and dehydration of)
                                                    147578-76-5P
                                                                      147578-77-6P
                     147578-74-3P
                                     147578-75-4P
     141848-52-4P
IT
                                                                      147578-82-3P
                                      147578-80-1P
                                                      147578-81-2P
                     147578-79-8P
     147578-78-7P
     147607-61-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and interlayer distances of)
     126013-69-2P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and interlayer spacing of)
                    34335-09-6P
     34001-96-2P
IT .
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation, interlayer spacing and intercalation of alkylamines into)
     ANSWER 60 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     147578-79-8 REGISTRY
Entered STN: 14 May 1993
RN
ED
     Copper, [phenylphosphonato(2-)-0]bis(1-propanamine)- (9CI) (CA INDEX
CN
     NAME)
     C12 H23 Cu N2 O3 P
MF
     CCS
CI
     CA
SR
     STN Files:
                   CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                 Ring
Analysis | Sequence | the Rings | Formula | Identifier | Occurrence
                                                        Count
                                     RF
                                                 RID
                     | SZ
             ES
   EΑ
                    =+=========
======
                                             146.150.18 | 1
                                |C6
                     16
         |C6
C6
```

# REFERENCE 1

AN 118:234154 CA
TI Intercalation of alkylamines into layered copper phosphonates
AU Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
Chemistry of Materials (1993), 5(4), 495-9

```
CODEN: CMATEX; ISSN: 0897-4756
DT
        Journal
        English
LA
        29-7 (Organometallic and Organometalloidal Compounds)
        Dehydration of layered copper phosphonates Cu(O3PR) H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase
CC
       C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate. Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(O3PCH3) and Cu(O3PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(O3PCH3) (RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of
        53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates intercalation alkylamine layered dehydrated copper phosphonate; inclusion
ST
        reaction alkylamine layered copper phosphonate
        Amines, reactions
IT
        RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl, intercalation of, into layered copper phosphonates)
Inclusion reaction
IT
        (intercalation, of alkylamines into layered copper phosphonates) 107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 111
IT
                                                                            111-86-4P, Octylamine
                              111-68-2P, 1-Heptanamine
         Hexylamine
         RL: PREP (Preparation)
               (intercalation of, into layered copper phosphonates)
86-30-9 71803-57-1 147578-73-2
IT
         RL: RCT (Reactant); RACT (Reactant or reagent)
         (interlayer spacing and dehydration of) 141848-52-4P 147578-74-3P 147578-75-4P
                                                                                        147578-76-5P
                                                                                                                  147578-77-6P
                                                             147578-75-4P
IT
                                                                                                                  147578-82-3P
                                                                                       147578-81-2P
                                                             147578-80-1P
                                   147578-79-8P
         147578-78-7P
         147607-61-2P
         RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and interlayer distances of)
         126013-69-2P
IT
         RL: SPN (Synthetic preparation); PREP (Preparation)
               (preparation and interlayer spacing of)
         34001-96-2P 34335-09-6P
IT
         RL: SPN (Synthetic preparation); PREP (Preparation)
               (preparation, interlayer spacing and intercalation of alkylamines into)
         ANSWER 61 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
         147578-74-3 REGISTRY
RN
         Copper, [methylphosphonato(2-)-0](1-propanamine)- (9CI) (CA INDEX NAME) C4 H12 Cu N O3 P
         Entered STN: 14 May 1993
ED
CN
MF
CI
         CCS
SR
         CA
         STN Files:
                                CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
n-Pr-NH2-Cu-0-P-Me
```

REFERENCE 1

# 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
118:234154 CA
AN
       Intercalation of alkylamines into layered copper phosphonates
TI
       Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
ΑU
       Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA Chemistry of Materials (1993), 5(4), 495-9
CODEN: CMATEX; ISSN: 0897-4756
CS
50
       Journal
DT
       English
LA
       29-7 (Organometallic and Organometalloidal Compounds)
CC
       Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 A in interlayer spacing compared to its monohydrate.
AB
       or more than 1 A in interlayer spacing compared to its monohydrate. Primary amines ChH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(03PCH3) and Cu(03PCH5). The copper methylphosphonate takes up 1 mol of amine forming Cu(03PCH3) (RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of
       53° with respect to the mean plane of the layer. The behavior of
       copper phosphonates was compared to those of Mn, Co, and Zn phosphonates.
       intercalation alkylamine layered dehydrated copper phosphonate; inclusion
ST
        reaction alkylamine layered copper phosphonate
       Amines, reactions
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
            (alkyl, intercalation of, into layered copper phosphonates)
        Inclusion reaction
IT
            (intercalation, of alkylamines into layered copper phosphonates)
       107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 111-68-2P, 1-Heptanamine 111-86-4P, Octylamine
IT
                                                                                                           111-26-2P,
       RL: PREP (Preparation)
(intercalation of, into layered copper phosphonates)
45986-30-9 71803-57-1 147578-73-2
IT
        RL: RCT (Reactant); RACT (Reactant or reagent)
             (interlayer spacing and dehydration of)
                                                                                                     147578-77-6P
                                                                              147578-76-5P
                               147578-74-3P
                                                      147578-75-4P
        141848-52-4P
IT
                                                                             147578-81-2P
                                                                                                     147578-82-3P
                                                      147578-80-1P
        147578-78-7P
                               147578-79-8P
        147607-61-2P
        RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and interlayer distances of)
IT
        126013-69-2P
        RL: SPN (Synthetic preparation); PREP (Preparation)
              preparation and interlayer spacing of)
                             34335-09-6P
IT
        34001-96-2P
        RL: SPN (Synthetic preparation); PREP (Preparation)
            (preparation, interlayer spacing and intercalation of alkylamines into)
        ANSWER 62 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        141848-52-4 REGISTRY
Entered STN: 19 Jun 1992
RN
ED
       Copper, (1-butanamine)[methylphosphonato(2-)-0]- (9CI) (CA INDEX NAME)
CN
        C5 H14 Cu N 03 P
MF
       CCS
CI
       CA
SR
        STN Files: CA, CAPLUS
LC
```

DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation)

$$n-Bu-NH_2-Cu-2+ 0-P-Me$$

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
118:234154 CA
AN
          Intercalation of alkylamines into layered copper phosphonates
          Zhang, Yiping; Scott, Karen J.; Clearfield, Abraham
Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
Chemistry of Materials (1993), 5(4), 495-9
CODEN: CMATEX; ISSN: 0897-4756
TI
ΑU
CS
SO
          Journal
DT
          English
LA
          29-7 (Organometallic and Organometalloidal Compounds)
          Dehydration of layered copper phosphonates Cu(O3PR)·H2O (R = CH3, C6H5, CH2C6H5) yields layered anhydrous salts Cu(O3PR) which show an increase of more than 1 Å in interlayer spacing compared to its monohydrate.

Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous cu(O3PCH3) and Cu(O3PCH5). The copper methylphosphonate takes up 1 mol
CC
AB
         Primary amines CnH2n+1NH2 (n = 3-8) were intercalated into anhydrous Cu(03PCH3) and Cu(03PC6H5). The copper methylphosphonate takes up 1 mol of amine forming Cu(03PCH3)·(RNH2), while 2 mol of amines were absorbed by copper phenylphosphonate. A plot of the interlayer distances of the intercalates vs. the number of carbon atoms in the alkyl chain gives a straight line with a slope of 2.01 Å, which indicates that the alkyl chains of amine are packed as double layers with a tilt angle of 53° with respect to the mean plane of the layer. The behavior of copper phosphonates was compared to those of Mn, Co, and Zn phosphonates intercalation alkylamine layered dehydrated copper phosphonate: inclusion
          intercalation alkylamine layered dehydrated copper phosphonate; inclusion reaction alkylamine layered copper phosphonate
ST
          Amines, reactions
RL: RCT (Reactant); RACT (Reactant_or reagent)
IT
                 (alkyl, intercalation of, into layered copper phosphonates)
           Inclusion reaction
IT
                 (intercalation, of alkylamines into layered copper phosphonates)
          107-10-8P, Propylamine, preparation 107-11-9P, 2-Propen-1-amine 109-73-9P, Butylamine, preparation 110-58-7P, 1-Pentanamine 114-88-2P, 1-Heptanamine 111-86-4P, Octylamine
IT
                                                                                                                                                  111-26-2P,
                 (intercalation of, into layered copper phosphonates) 86-30-9 71803-57-1 147578-73-2
          RL: PREP (Preparation)
IT
          RL: RCT (Reactant); RACT (Reactant or reagent)
(interlayer spacing and dehydration of)
                                                                                                                                          147578-77-6P
                                                                                                          147578-76-5P
                                                                          147578-75-4P
           141848-52-4P
                                          147578-74-3P
IT
                                                                                                                                          147578-82-3P
                                                                          147578-80-1P
                                                                                                          147578-81-2P
                                          147578-79-8P
           147578-78-7P
           147607-61-2P
           RL: SPN (Synthetic preparation); PREP (Preparation)
                  (preparation and interlayer distances of)
           126013-69-2P
IT
          RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and interlayer spacing of)
                                     34335-09-6P
           34001-96-2P
IT
```

```
(preparation, interlayer spacing and intercalation of alkylamines into)
REFERENCE 2
       117:19105 CA
AN
       Synthesis, crystal structures, and coordination intercalation behavior of
TI
       two copper phosphonates
       Zhang, Yiping; Clearfield, Abraham
       Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA Inorganic Chemistry (1992), 31(13), 2821-6
CODEN: INOCAJ; ISSN: 0020-1669
ΑU
CS
50
DT
       Journal
       English
LA
       78-5 (Inorganic Chemicals and Reactions)
CC
       Section cross-reference(s): 75
       Cu(03PMe).H20 and Cu(03PPh).H20 were synthesized and their structures
       determined Cu(03PMe).H20 is monoclinic: space group P21/c, a 8.495(4), b 7.580(4), c 7.289(4) Å, β 90.08 (4)°, Z = 4, R = 0.030, Rw = 0.041. The structure is layered as formed by unusual 5-coordinate distorted tetragonal pyramidal Cu atoms. One 0 of each phosphonate bonds to 2 Cu atoms forming a chain, while the other 2 phosphonate 0 atoms bond to 2 Cu atoms in an adjacent chain. The base of the pyramid consists of 3 phosphonate 0 atoms and the coordinated H20 mol All H bonds are of the
AB
       phosphonate O atoms and the coordinated H2O mol. All H bonds are of the
       intralayer type, so only van der Waals forces exist between adjacent
       layers. Amines are coordinatively intercalated with layer expansion. Cu(03PPh).H20 is orthorhombic: space group Pbca, a 7.5547(4), b 7.4478(6),
       c 27.928(1) Å, Z = 8, R = 0.037 and Rw = 0.043. The coordination about the Cu atoms and the layer structure are identical to those of the
       O3PMe compound The Ph rings in the interlamellar space are oriented at a
       98° angle to each other in adjacent rows. These structures are compared to those of other layered divalent phosphonates and Cu
       phosphites.
       crystal structure copper phosphonate; amine intercalation copper
ST
       phosphonate
       Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
IT
            (intercalation of, in anhydrous and hydrous copper phosphonate)
       Crystal structure
IT
       Molecular structure
            (of copper phosphonate hydrates)
       Inclusion reaction
IT
            (intercalation, of amine in anhydrous and hydrous copper phosphonate)
       109-73-9, Butylamine, reactions
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
            (intercalation of, in anhydrous and hydrous copper phosphonate)
       71803-57-1P
IT
       RL: SPN (Synthetic preparation); PREP (Preparation)
            (preparation and crystal structure and intercalation reaction of, with
            amine)
       72702-21-7P
IT
       RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
            (preparation and crystal structure of)
                             141848-53-5P
IT
       141848-52-4P
       RL: SPN (Synthetic preparation); PREP (Preparation)
       (preparation and interlayer spacing of intercalation compound)
993-13-5, Methylphosphonic acid 1571-33-1, Phenylphosphonic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
IT
       (reaction of, with cupric sulfate in presence of hydrolyzing urea) 7758-98-7, Cupric sulfate, reactions
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
```

RL: SPN (Synthetic preparation); PREP (Preparation)

(reaction of, with phosphonic acids in presence of hydrolyzing urea)

1.35

```
ANSWER 63 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      138521-45-6 REGISTRY
RN
      Entered STN: 24 Jan 1992
      Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-0]-, tribromide, (OC-6-23)- (9CI) (CA INDEX NAME)
ED
CN
      C3 H23 C0 N5 O S . 3 Br
MF
      CCS
CI
SR
      CA
                     CA, CAPLUS.
LC
      STN Files:
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation)
     (138521-43-4)
```

●3 Br-

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
116:50338 CA
      Synthesis and characterization of trans-[Co(NH3)4(NH2CH3)L]3+[L=
ΤI
      (CH3)2SO or (CH3)2NCHO] complexes
      Sienra, Beatriz; Massaferro, Adriana
ΑU
      Fac. Quim., Montevideo, Urug. Polyhedron (1991), 10(17), 2075-8 CODEN: PLYHDE; ISSN: 0277-5387
CS
S0
      Journal
DT
      English
LA
      78-7 (Inorganic Chemicals and Reactions)
CC
      trans-[Co(NH3)4(NH2Me)Me2SO]X3 (X = Clo4, Br) and trans-
AB
      [CO(NH3)4(NH2Me)Me2NCHO](ClO4)3 are prepared by Ag+-induced solvolysis of trans-[Co(NH3)4(NH2Me)X]2+ (X = Cl or Br) complexes in DMSO or DMF. The complexes were characterized by electronic, IR and 1H NMR. DMSO and DMF
      are bonded through the oxygen atom. The trans-complexes obtained are not
      contaminated with the cis-isomers.
      cobalt amine ammine DMF DMSO complex
ST
      134066-28-7
TT
      RL: RCT (Reactant); RACT (Reactant or reagent) (dechlorination of, in DMSO)
      91321-36-7
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
           (dechlorination of, in DMSO or DMF)
                         138521-45-6P 138521-47-8P
      138521-44-5P
IT
```

```
RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     ANSWER 64 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     138521-44-5 REGISTRY
RN
     Entered STN: 24 Jan 1992
ED
     Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-0]-, (OC-6-23)-,
CN
     triperchlorate (9CI) (CA INDEX NAME)
     C3 H23 CO N5 O S . 3 C1 O4
MF
     CA
SR
     STN Files:
                  CA, CAPLUS
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation)
           1
     CM
          138521-43-4
     CRN
     CMF C3 H23 CO N5 O S
     CCI CCS
             NH3
      H<sub>3</sub>N
Me-NH2
      H3N
           2
     CM
           14797-73-0
      CRN
           cl 04
      CMF
                 1 REFERENCES IN FILE CA (1907 TO DATE)
                 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      116:50338 CA
AN
      synthesis and characterization of trans-[Co(NH3)4(NH2CH3)L]3+[L=
TI
      (CH3)2SO or (CH3)2NCHO] complexes
      Sienra, Beatriz; Massaferro, Adriana
ΑU
      Fac. Quim., Montevideo, Urug. Polyhedron (1991), 10(17), 2075-8 CODEN: PLYHDE; ISSN: 0277-5387
CS
SO
      Journal
DT
LA
      English
      78-7 (Inorganic Chemicals and Reactions)
CC
```

```
trans-[Co(NH3)4(NH2Me)Me2SO]X3 (X = ClO4, Br) and trans-
AB
     [Co(NH3)4(NH2Me)Me2NCHO](Cl04)3 are prepared by Ag+-induced solvolysis of
     trans-[CO(NH3)4(NH2Me)X]2+(X=Cl or Br) complexes in DMSO or DMF. The complexes were characterized by electronic, IR and 1H NMR. DMSO and DMF
     are bonded through the oxygen atom. The trans-complexes obtained are not
     contaminated with the cis-isomers.
     cobalt amine ammine DMF DMSO complex
ST
     134066-28-7
IT.
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (dechlorination of, in DMSO)
     91321-36-7
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (dechlorination of, in DMSO or DMF)
                     138521-45-6P
                                        138521-47-8P
     138521-44-5P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     ANSWER 65 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     138521-43-4 REGISTRY
RN
     Entered STN: 24 Jan 1992
     Cobalt(3+), tetraammine(methanamine)[(sulfinyl-k0)bis[methane]]-, (OC-6-23)- (9CI) (CA INDEX NAME)
ED
CN
     Cobalt(3+), tetraammine(methanamine)[sulfinylbis[methane]-0]-, (OC-6-23)-C3 H23 Co N5 O S
OTHER CA INDEX NAMES:
CN
MF
     CCS, COM
CI
SR
     CA
                     CA, CAPLUS
     STN Files:
LC
       CAplus document type: Journal
DT.CA
        Roles from non-patents: PROC (Process); PRP (Properties); RACT
RL.NP
        (Reactant or reagent)
      H<sub>3</sub>N
              NH3
              3+
Me-NH2
      H<sub>3</sub>N
                 Me-
                 1 REFERENCES IN FILE CA (1907 TO DATE)
                 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      132:142592 CA
      Variable temperature and pressure study of the aquation reactions of
ΤÏ
      cobalt(III) and chromium(III) penta- and tetra-amines
      Benzo, Fabian; Bernhardt, Paul V.; Gonzalez, Gabriel; Martinez, Manuel;
ΑU
      Sienra, Beatriz
      Facultad de Quimica, Catedra de Quimica Inorganica, Universidad de la
CS
      Republica, Montevideo, 11800, Urug.

Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry
SO
      (1999), (22), 3973-3979
CODEN: JCDTBI; ISSN: 0300-9246
Royal society of Chemistry
PB
      Journal
DT
```

```
LA
        67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
CC
        Section cross-reference(s): 78
        Preparation of a series of specific penta- and tetra-amine derivs. of CoIII and CrIII with a neutral leaving ligand has been carried out in order to
AB
        accomplish a fine tuning of the associativeness/dissociativeness of their
        substitution reactions. Spontaneous aquation reactions of the neutral
        ligands have been studied at variable temperature and pressure. Although rate
        consts. and thermal activation parameters show an important degree of scatter, the values determined for the activation vols. of the substitution
        process illustrate the mechanistic fine tuning that may be achieved for
        these reactions. In all cases, in the absence of important steric
        constraints in the mol., electronic inductive effects seem to be the most
        important factor accounting for the dissociative shifts observed both for
       important factor accounting for the dissociative shifts observed both for pentaamine i.e. \Delta V.dbldag. = +4.0 or +14.0 cm3 mol-1 and +5.2 or +16.5 cm3 mol-1 for the aquation of cis- or trans-[Co(MeNH2)(NH3)4(DMF)]3+ and cis- or trans-[CoL15(DMF)]3+ resp., where L15 represents a pentaamine macrocyclic ligand, tetraamine systems i.e. \Delta V.dbldag. = +4.1 or +8.4 cm3 mol-1 and -10.8 or -7.4 cm3 mol-1 for the aquation of cis-[Co(NH3)4Cl(DMAC)]2+ (DMAC = dimethylacetamide) or cis-[Co(en)2Cl(DMAC)]2+ and cis-[Cr(NH3)4Cl(DMF)]2+ or cis-[Cr(en)2Cl(DMF)]2+. From the results, clear evidence is obtained which indicates that, only when the situation is borderline Ia/Id, or the steric demands are increased dramatically, dissociative shifts are observed; in all other cases electronic inductive effects seem to be dominant for such a tuning of the substitution process.
        such a tuning of the substitution process.
        cobalt amine complex aquation variable temp pressure; chromium amine
ST
        complex aquation variable temp pressure
        Activation enthalpy
IT
        Activation entropy
        Activation volume
        Aquation
        Aquation kinetics
             (variable temperature and pressure study of aquation reactions of
cobalt(III)
             and chromium(III) penta- and tetra-amines)
                                                                                           46240-37-3
                                                                      19066-42-3
                                                 15696-65-8
                             15696-64-7
        15696-63-6
IT
                                                                                           62728-63-6
                                                                      62728-54-5
                                                  62728-47-6
        59301-98-3
                             62728-45-4
                                                                        138521-46-7
                                                                                              256652-23-0
        72382-37-7
                            72382-38-8
                                                 138521-43-4
                                                                                                  256652-34-3
                                                                           256652-32-1
                                                     256652-30-9
                              256652-28-5
        256652-25-2
                                                                                                  256652-43-4
                                                     256652-39-8
                                                                           256652-41-2
                              256652-37-6
        256652-35-4
                              256652-47-8
                                                                                                 256656-90-3
                                                                           256656-89-0
                                                     256652-51-4
        256652-45-6
                              256656-96-9
        256656-91-4
        RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
             (variable temperature and pressure study of aquation reactions of
cobalt(III)
             and chromium(III) penta- and tetra-amines)
                      THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD
             51
(1) Baldwin, M; J Chem Soc 1961, P4637 CAPLUS
(2) Balt, S; Transition Met Chem 1984, V9, P224 CAPLUS (3) Benzo, F; J Chem Crystallogr 1998, V28, P69 CAPLUS
 (4) Benzo, F; Polyhedron 1996, V15, P1915 CAPLUS
 (5) Benzo, F; to be published
 (6) Benzo, F; to be published
(7) Binstead, R; Specfit 1993
(8) Bruce, H; Inorg Chem 1987, V26, P4024
(9) Comba, P; Coord Chem Rev 1999, V182, P343
(10) Crespo, M; J Chem Soc, Dalton Trans 1997, P1321
(11) Curtis, N; Inorg Chem 1986, V25, P1033 CAPLUS
(12) Curtis, N; Inorg Chem 1989, V28, P329 CAPLUS
```

```
(13) Ghosh, M; Coord Chem Rev 1988, V91, P1 CAPLUS (14) Gonzalez, G; Inorg Chem 1994, V33, P2330 CAPLUS (15) Gonzalez, G; Inorg Chim Acta 1993, V203, P229 CAPLUS (16) Conzalez, G; I Chem Sec. Politon Trans 1995, P291 CAPLUS
 (16) Gonzalez, G; J Chem Soc, Dalton Trans 1995, P891 CAPLUS (17) Hall, S; The XTAL 3.2 User's Manual 1992
(18) Heatherington, A; Inorg Chim Acta 1980, V44, PL279
(18) Heatnerington, A; Inorg Chim Acta 1980, V44, PL2/9
(19) Hoppenjans, D; Inorg Chem 1968, V7, P2506 CAPLUS
(20) House, D; Comments Inorg Chem 1997, V19, P326
(21) House, D; J Inorg Nucl Chem 1966, V28, P904 CAPLUS
(22) Kitamura, Y; Inorg Chem 1986, V25, P3887 CAPLUS
(23) Kitamura, Y; Inorg Chim Acta 1989, V159, P181 CAPLUS
(24) Kitamura, Y; Inorg Chim Acta 1989, V156, P31 CAPLUS
(25) Lantzke, I; Aust J Chem 1966, V19, P949 CAPLUS
(26) Lawrance, G: Aust J Chem 1980, V33, P273 CAPLUS
(25) Lantzke, 1; Aust J Chem 1900, V13, F343 CAPLUS

(26) Lawrance, G; Aust J Chem 1980, V33, P273 CAPLUS

(27) Lawrance, G; Inorg Chem 1982, V21, P3687 CAPLUS

(28) Lawrance, G; Inorg Synth 1986, V24, P250 CAPLUS

(29) Lawrance, G; J Chem Soc, Dalton Trans 1992, P1635 CAPLUS
 (30) Lawrance, G; J Chem Soc, Dalton Trans 1992, P1643
 (31) Lawrance, G; J Chem Soc, Dalton Trans. 1992, P823 CAPLUS
(31) Lawrance, G; J Chem Soc, Dalton Trans. 1992, P823. CAPLUS
(32) Lay, P; Coord Chem Rev 1991, V110, P213 CAPLUS
(33) Lay, P; Inorg Chem 1987, V26, P2144 CAPLUS
(34) Malek, D; J Inorg Nucl Chem 1980, V42, P1313 CAPLUS
(35) Martinez, M; J Chem Soc, Dalton Trans 1995, P4107 CAPLUS
(36) Monsted, L; Coord Chem Rev 1989, V94, P109
(37) Palmer, D; Aust J Chem 1967, V20, P53 CAPLUS
(38) Palmer, D; Aust J Chem 1968, V21, P2895 CAPLUS
(39) Poth, T; Eur J Inorg Chem 1999, P643 CAPLUS
(40) Rigg, J; J Inorg Nucl Chem 1965, V27, P653 CAPLUS
(41) Rindermann, W; Inorg Chim Acta 1982, V64, PL203 CAPLUS
(42) Seligson. A: J Am Chem Soc 1991, V113, P2520 CAPLUS
 (42) Seligson, A; J Am Chem Soc 1991, V113, P2520 CAPLUS
(43) Sheldrick, G; Acta Crystallogr, Sect A 1990, V46, P467
(44) Sheldrick, G; SHELX97, Program for Crystal Structure Determination 1997
(45) Spek, A; Acta Crystallogr, Sect A 1990, V46, PC34
(46) Springborg, J; Inorg Synth 1987, V18, P75
(47) Swaddle, T; Comments Inorg Chem 1991, V12, P237 CAPLUS
(48) Tobe, M; Inorganic Reaction Mechanisms 1999
(49) Tobe M: 1 Chem Soc 1964 P2991 CAPLUS
                                J Chem Soc 1964, P2991 CAPLUS
  (49) Tobe, M;
 (50) van Eldik, R; Inorganic High Pressure Chemistry: Kinetics and Mechanisms
          1986
 (51) Wilkins, R; Kinetics and Mechanisms of Reactions of Transition Metal
          Complexes 1991
             ANSWER 66 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
 L9
             134066-33-4 REGISTRY
 RN
             Entered STN: 07 Jun 1991
 ED
            Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-0]-, (OC-6-23)-, nitrate (9CI) (CA INDEX NAME)
 CN
OTHER CA INDEX NAMES:
             sulfurous acid, cobalt complex
            trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
             C H17 CO N5 O3 S . N O3
MF
             CA
 SR
             STN Files:
                                           CA, CAPLUS
 DT.CA CAplus document type: Journal
 RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
             CM
             CRN
                        134066-32-3
                        C H17 Co N5 O3 S
             CMF
```

```
Page 208
```

CCI CCS

CM 2

CRN 14797-55-8 CMF N 03

0 || 0== N- 0-

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

114:258445 CA AN synthesis, characterization and some reactions of trans-TT tetraamminebromo(methanamine)cobalt(2+) and transtetraammine(methanamine(nitratocobalt(2+)\_complexes Sienra, B.; Massaferro, A.; Piriz Mac-Coll, C. R. ΑU Univ. Republica, Montevideo, Urug. Zeitschrift fuer Anorganische und Allgemeine Chemie (1990), 590, 222-8 CS SO CODEN: ZAACAB; ISSN: 0044-2313 Journal DT English LA 78-7 (Inorganic Chemicals and Reactions) CC The preparation of trans-[Co(NH3)4(CH3NH2)Br]2+ (I) and trans-[Co(NH3)4(CH3NH2)(NO3)]2+ is described. The UV-visible spectra of the AB complexes indicate a decrease of the ligand field compared to the parent pentaammines. IR spectra match with the pattern of the corresponding The catalyzed (by Hg2+) aquation of I occurred with pentaammines. retention of the stereochem. configuration. The base hydrolysis (studied at 25°) products show trans to cis rearrangement for both complexes. 1H NMR spectroscopy is used for identification of the stereochem. configuration of the compds. aquation cobalt ammine methanamine bromo complex; hydrolysis cobalt ammine ST methanamine complex isomerization; cobalt ammine methanamine complex **Isomerization** IT (in base hydrolysis of cobalt ammine methylamine complexes) IT (mercuric-catalyzed, of cobalt ammine methylamine complexes) Hydrolysis IT

```
(base, of cobalt ammine methylamine complexes, isomerization in) 134108-63-7P, cis-Tetraammineaqua(methylamine)cobalt(3+)
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation)
         (formation of, in base hydrolysis of trans bromo complex with
         isomerization)
     134066-35-6P, trans-Tetraammineaqua(methylamine)cobalt(2+) perchlorate
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in catalyzed aquation of bromo complex)
     91321-36-7, trans-Tetraamminechloro(methylamine)cobalt(2+) perchlorate
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (mercuric-catalyzed aquation and reaction of, with mercuric nitrate)
     134066-29-8P, trans-Tetraamminebromo(methylamine)cobalt(2+) dibromide
IT
     134066-31-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and anion exchange of)
     134096-89-2P, trans-Tetraammine(methylamine)nitratocobalt(2+) perchlorate
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (preparation and base hydrolysis of)
     134066-33-4P, trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
     (preparation and decomposition of, in presence of nitric acid)
134066-28-7P, trans-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
RL: SPN (Synthetic preparation); PREP (Preparation)
IT
         (preparation and mercuric-catalyzed aquation and base hydrolysis of)
     100788-48-5P, trans-Tetraammineaqua(methylamine)cobalt(3+) perchlorate
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (preparation and reaction of, with bromide)
     134066-26-5P, trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (preparation and reaction of, with hydrogen bromide)
     134108-62-6P, cis-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     88587-77-3, trans-Tetraamminehydroxysulfitocobalt
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with methylamine bromide)
     ANSWER 67 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     134066-32-3 REGISTRY
RN
     Entered STN: 07 Jun 1991
ED
     Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-\kappa0]-, (OC-6-23)-(9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
     Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-0]-, (OC-6-23)-
CN
     sulfurous acid, cobalt complex
C H17 Co N5 O3 S
CN
MF
     CCS, COM
CI
     CA
SR
     STN Files:
                    CA, CAPLUS
LC
DT.CA CAplus document type: Journal
       Roles from non-patents: RACT (Reactant or reagent)
```

```
133:79995 CA
AN
      Inductive effect of methyl groups on acidopentaaminecobalt(III) complexes
TI
      Benzo, Fabian; Beyer, Lothar; Bozoglian, Fernando; Hallmeier, Karl-Heinz;
ΑU
       Sienra, Beatriz
      Universidad de la Republica, Catedra de Quimica Inorganica, Montevideo,
CS
       Polyhedron (2000), 19(8), 971-974
S<sub>0</sub>
       CODEN: PLYHDE; ISSN: 0277-5387
       Elsevier Science Ltd.
PB
       Journal
DT
ΙΔ
       67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
       English
CC
       Section cross-reference(s): 78
       Electron spectroscopy for chemical anal. (ESCA) was performed for [Co(NH3)5Cl](ClO4)2, trans-[Co(NH3)4(NH2CH3)Cl]-(ClO4) 2, [Co(NH2CH3)5Cl](ClO4)2 and trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4)
AB
                      Comparison of the results for the complexes
       [Co(NH3)5Cl](ClO4)2 and trans-[Co(NH3)4(NH2CH3)Cl](ClO4)2 shows clearly the electronic influence (+I effect) of the methylamine group on the
       cobalt and through this on the chlorine atom in trans position.
       Comparison of [Co(NH2CH3)5Cl](Cl04)2 with trans-
[Co(NH3)4(NH2CH3)Cl](Cl04)2 shows that methylation of the four cis-NH3
ligands does not produce a proportional decrease in the binding energy of
       the cobalt atom, while the electron d. of the chloro ligand is not affected. For the complex trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4) the +I
       effect is almost completely compensated by the presence of the sulfato
       group in trans position. Acid dissociation consts. are also reported for [Co(NH3)5(OH2)]3+ and trans-[Co(NH3)4(NH2CH3)(OH2)]3+ ions. The implications of these results for the mechanism of the acid and base
       hydrolysis reactions of acidopentaaminecobalt(III) complexes are
       discussed. The preparation of the trans-[Co(NH3)4(NH2CH3)(OSO3)](Cl O4)
       complex through the trans-[Co(NH3)4(NH2CH3)(SO3)]+ precursor is also
       described.
       inductive effect methyl group acido amine cobalt complex
ST
IT
       Hydrolysis
           (acid, mechanism; inductive effect of Me groups on
           acidopentaaminecobalt(III) complexes)
       Dissociation constant
IT
           (acid; inductive effect of Me groups on acidopentaaminecobalt(III)
           complexes)
IT
       Hydrolysis
            (base, mechanism; inductive effect of Me groups on
```

```
acidopentaaminecobalt(III) complexes)
            Inductive effect
IT
           Methyl group
                   (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
                                                                     91321-36-7
                                                                                                  279674-00-9
                                         15392-60-6
            15156-18-0
IT
            RL: PRP (Properties)
                   (inductive effect of Me groups on acidopentaaminecobalt(III) complexes)
                                        68250-09-9
                                                                      134066-32-3
            14403-82-8
IT
           RL: RCT (Reactant); RACT (Reactant or reagent)

(inductive effect of Me groups on acidopentaaminecobalt(III) complexes)

IT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Balt, S; J Chem Soc, Dalton Trans 1983, P2415 CAPLUS (2) Balt, S; Transition Met Chem 1984, V9, P224 CAPLUS (3) Benzo, F; J Chem Crystallogr 1998, V28, P69 CAPLUS (4) Benzo, F; Polyhedron 1915, V15, P1996 (5) Benzo, F; to be published in Inorg React Mechanims
 (6) Benzo, F; to be published in J Chem Soc, Dalton Trans
 (7) Brasch, N; Inorg Chem 1989, V28, P4567 CAPLUS
(8) Buckingham, D; Inorg Chem 1970, V9, P1790 CAPLUS
(9) Buckingham, D; Inorg Chem 1970, V9, P655 CAPLUS
(10) Buckingham, D; J Am Chem Soc 1967, V89, P5129 CAPLUS
(11) Curtis N: Trong Chem 1986, V25, P1032 CAPLUS
(10) Buckingham, D; J Am Chem Soc 1967, V89, P5129 CAF

(11) Curtis, N; Inorg Chem 1986, V25, P1033 CAPLUS

(12) Curtis, N; Inorg Chem 1986, V25, P484 CAPLUS

(13) Curtis, N; Inorg Chem 1989, V28, P329 CAPLUS

(14) Dixon, N; Inorg Chem 1982, V21, P688 CAPLUS

(15) Foxman, B; Inorg Chem 1932, V17, P1978

(16) Gonzalez, G; Inorg Chem 1994, V33, P2330 CAPLUS

(17) Jackson, W; Inorg Chem 1984, V23, P2473 CAPLUS

(18) Jordan, R; Inorg Chem 1986, V35, P3725 CAPLUS

(19) Kitamura, Y; Inorg Chem 1989, V28, P333 CAPLUS

(20) Lawrence, G; Inorg Chem 1984, V23, P3922

(21) Lay, P; Inorg Chem 1987, V26, P2144 CAPLUS

(22) Massaferro, A; An Quim 1992, V88, P230 CAPLUS

(23) Nordmeyer, F; Inorg Chem 1969, V8, P2781

(24) Rotzinger, F; Inorg Chem 1988, V27, P768 CAPLUS

(25) Rotzinger, F; Inorg Chem 1988, V27, P772 CAPLUS

(26) Rotzinger, F; Inorg Chem 1988, V27, P772 CAPLUS

(27) Sienra, B; Polyhedron 1991, V30, P2763 CAPLUS

(28) Sienra, B; Z Anorg Allg Chem 1990, V590, P222 CAPLUS
 (28) Sienra, B; Z Anorg Allg Chem 1990, V590, P222 CAPLUS
 (29) Sisley, M; Inorg Chem 1981, V20, P2799 CAPLUS (30) Swaddle, T; Can J Chem 1977, V55, P3166 CAPLUS (31) Tobe, M; Inorganic Reaction Mechanisms 1999
 (32) Wilkins, R; Kinetics and Mechanism of Reactions of Transition Metal
          Complexes 1991
            ANSWER 68 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
 L9
            134066-26-5 REGISTRY
 RN
            Entered STN: 07 Jun 1991
 ED
            Cobalt(1+), tetraammine(methanamine)[sulfito(2-)-0]-, bromide, (OC-6-23)-
 CN
                            (CA INDEX NAME)
             (9CI)
OTHER CA INDEX NAMES:
            sulfurous acid, cobalt complex
            trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
            C H17 Co N5 03 S . Br
MF
            CCS
 CI
 SR
            CA
                                       CA, CAPLUS
            STN Files:
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
 CRN (134066-32-3)
```

● Br

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

114:258445 CA AN Synthesis, characterization and some reactions of trans-TI tetraamminebromo(methanamine)cobalt(2+) and transtetraammine(methanamine(nitratocobalt(2+) complexes Sienra, B.; Massaferro, A.; Piriz Mac-Coll, C. R. Univ. Republica, Montevideo, Urug. Zeitschrift fuer Anorganische und Allgemeine Chemie (1990), 590, 222-8 ΑU CS S0 CODEN: ZAACAB; ISSN: 0044-2313 Journal DT English LA 78-7 (Inorganic Chemicals and Reactions) The preparation of trans-[Co(NH3)4(CH3NH2)Br]2+ (I) and trans-[Co(NH3)4(CH3NH2)(NO3)]2+ is described. The UV-visible spectra of the complexes indicate a decrease of the ligand field compared to the parent pentaammines. IR spectra match with the pattern of the corresponding pentaammines. CC AB pentaammines. The catalyzed (by Hg2+) aquation of I occurred with retention of the stereochem. configuration. The base hydrolysis (studied at 25°) products show trans to cis rearrangement for both complexes. 1H NMR spectroscopy is used for identification of the stereochem. configuration of the compds. aquation cobalt ammine methanamine bromo complex; hydrolysis cobalt ammine ST methanamine complex isomerization; cobalt ammine methanamine complex Isomerization TT (in base hydrolysis of cobalt ammine methylamine complexes) IT Aquation (mercuric-catalyzed, of cobalt ammine methylamine complexes) Hydrolysis IT (base, of cobalt ammine methylamine complexes, isomerization in) 134108-63-7P, cis-Tetraammineaqua(methylamine)cobalt(3+) IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in base hydrolysis of trans bromo complex with isomerization) 134066-35-6P, trans-Tetraammineaqua(methylamine)cobalt(2+) perchlorate IT RL: FORM (Formation, nonpreparative); PREP (Preparation)

```
(formation of, in catalyzed aquation of bromo complex)
     91321-36-7, trans-Tetraamminechloro(methylamine)cobalt(2+) perchlorate
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (mercuric-catalyzed aquation and reaction of, with mercuric nitrate)
     134066-29-8P, trans-Tetraamminebromo(methylamine)cobalt(2+) dibromide
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation and anion exchange of)
     134096-89-2P, trans-Tetraammine(methylamine)nitratocobalt(2+) perchlorate
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (preparation and base hydrolysis of)
     134066-33-4P, trans-Tetraammine(methylamine)sulfitocobalt(1+) nitrate
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
     (preparation and decomposition of, in presence of nitric acid) 134066-28-7P, trans-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and mercuric-catalyzed aquation and base hydrolysis of)
     100788-48-5P, trans-Tetraammineaqua(methylamine)cobalt(3+) perchlorate
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
     (preparation and reaction of, with bromide)
134066-26-5P, trans-Tetraammine(methylamine)sulfitocobalt(1+) monobromide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
IT
      (Reactant or reagent)
         (preparation and reaction of, with hydrogen bromide)
     134108-62-6P, cis-Tetraamminebromo(methylamine)cobalt(2+) perchlorate
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
      88587-77-3, trans-Tetraamminehydroxysulfitocobalt
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with methylamine bromide)
     ANSWER 69 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN 126830-36-2 REGISTRY Entered STN: 27 Apr 1990
L9
RN
ED
     Zinc, bis(4-amino-N-2-pyrimidinylbenzenesulfonamidato)bis(methanamine)-,
CN
      (T-4)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
      Benzenesulfonamide, 4-amino-N-2-pyrimidinyl-, zinc complex
CN
      C22 H28 N10 O4 S2 Zn
MF
CI
      CCS
SR
      CA
                    CA, CAPLUS, TOXCENTER
      STN Files:
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
        PRP (Properties); USES (Uses)
Ring System Data
                                                   Ring
Elemental|Elemental| Size of |Ring System|
                                                                RID
Analysis | Sequence | the Rings | Formula | Identifier | Occurrence
                                                           Count
                                       RF
                                                   RID
   EΑ
               ES
                          SZ
                                                  ---------
|46.150.18 |2
                                  C6
           C6
                      16
C6
                                               146.195.39 12
                                  C4N2
                      16
C4N2
           INCNC3
```

```
123:102111 CA
AN
       Zinc sulfadiazines: novel topical antimicrobial agents for burns
TI
       Lee, A. R.; Huang, W. H.
ΑU
       Sch. Pharmacy, National Defense Med. Cent., Taipei, Taiwan
CS
       Journal of Pharmacy and Pharmacology (1995), 47(6), 503-9
S0
       CODEN: JPPMAB; ISSN: 0022-3573
Royal Pharmaceutical Society of Great Britain
PB
        Journal
DT
       English
1-5 (Pharmacology)
LA
CC
        Two new zinc sulfadiazine (Zn(SD)2)-amine complexes, zinc
       sulfadiazine-methylamine (Zn(SD)2(CH3NH2)2) and zinc sulfadiazine-
       ethylenediamine (Zn(SD)2(C2H8N2)3.H2O), were prepared and compared with silver sulfadiazine (AgSD). The compds. were readily obtained by reaction
       of zinc nitrate hexahydrate with sulfadiazine or its methylamine and ethylenediamine salts. Structure was established by X-ray crystallog. and UV-visible, IR and NMR spectroscopy. The products were effective, in-vitro, against Gram-pos. and Gram-neg. bacteria as well as fungus. However, their activity is partially reversed by p-aminobenzoic acid. Further investigations in burned mice revealed that these compds.
        displayed a potential value in the prevention and treatment of wound healing, and diminution of mortality and weight loss. The toxicity of
        Zn(SD)2 derivs. was much lower than that of AgSD. The better aqueous
solubility
       and skin permeability may explain the reason for their superiority over AgSD in the efficacy for topical therapy. Zn(SD)2(CH3NH2)2 was consistently more potent and was chosen for further development in clin.
                  The similarity in complexation between Sn(SD)2(CH3NH2)2 and AgSD
        may be significant to distinguish that from any other Zn(SD)2 derivative in
        bioactivity.
        antimicrobíal zinc sulfadiazine amine complex burn
ST
IT
        Biocides
              (zinc sulfadiazines and novel topical antimicrobial agents for burns)
                                                                                               10196-18-6, Zinc
                                             547-32-0, Sulfadiazine sodium
        68-35-9, Sulfadiazine
IT
        nitrate hexahydrate
        RL: RCT (Reactant); RACT (Reactant or reagent)
              (zinc sulfadiazines and novel topical antimicrobial agents for burns)
                               126830-36-2P
        126830-35-1P
IT
        RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(zinc sulfadiazines and novel topical antimicrobial agents for burns)
```

```
112:209715 CA
AN
     A facile synthesis of zinc sulfadiazine derivatives
TI
     Lee, An Rong; Huang, Wen Hsin; Lai, Jin Shing; Chan, Shu Fei
ΑU
     Sch. Pharm., Natl. Def. Med. Cent., Taipei, Taiwan
Zhonghua Yaoxue Zazhi (1989), 41(4), 345-8
CS
S<sub>0</sub>
     CODEN: CYHCEX; ISSN: 1016-1015
     Journal
DT
     English
LA
     78-7 (Inorganic Chemicals and Reactions)
CC
     Section cross-reference(s): 28
     Treatment of sulfadiazine with Zn(NO3)2 in the presence of NH4OH, MeNH2,
AB
     or H2NCH2CH2NH2 gave the corresponding title complexes, whose mol.
     structures were determined
     zinc sulfadiazine amine complex; mol structure zinc sulfadiazine complex
ST
     Molecular structure
IT
         (of zinc-sulfadiazine-amine complexes)
     7779-88-6, Zinc nitrate
IT
     RL: RCT (Reactant); RACT (Reactant or reagent) (complexation of, with sulfadiazine and ammonia, methylamine, or
         ethylenediamine)
     68-35-9, Sulfadiazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with zinc nitrate and ammonia, methylamine, or
IT
         ethylenediamine)
                                      126830-36-2P
                     126830-35-1P
     88667-78-1P
IT
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (preparation and mol. structure of)
     ANSWER 70 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     110946-24-2 REGISTRY
RN
     Entered STN: 24 Oct 1987
ED
     Mercury, bis(1-butanamine-N)bis(thiocyanato-S)-, (T-4)- (9CI) (CA INDEX
CN
      NAME)
OTHER CA INDEX NAMES:
     1-Butanamine, mercury complex C10 H22 Hg N4 S2
CN
MF
CI
      CCS
SR
      CA
                    CA, CAPLUS
     STN Files:
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)
                  Hg-NH2-Bu-n
n-Bu-NH2-
                   S--- CN
                 1 REFERENCES IN FILE CA (1907 TO DATE)
                 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      107:184014 CA
ΑN
      Study of the bond strength in complex compounds by proton NMR
TI
      Galitskaya, S. M.; Pavlenko, L. I.
ΑU
CS
      USSR
```

```
Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
SO
     CODEN: VLPIAZ; IŠSN: 0460-0436
     Journal
DT
     Russian
LA
     65-5 (General Physical Chemistry)
CC
     Section cross-reference(s): 77
     Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN,
     NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases
AB
     in the order CN > NCS # NCSe.
     bond energy complex NMR; zinc butylamine cyano complex bond energy; thiocyanato butylamine cadmium complex bond energy; selenocyanato
ST
     butylamine cadmium complex bond energy; cadmium butylamine cyano complex
     bond energy; mercury butylamine cyano complex bond energy
     Bond energy
IT
         (in Group IIB metal complexes, NMR in study of)
     Nuclear magnetic resonance
IT
         (of Group IIB metal complexes)
                                  32491-88-6 38255-54-8 38271-02-2
                   32491-84-2
     32491-81-9
IT
                                    110946-25-3
                                                   110987-94-5
                    110946-24-2
     110945-33-0
     RL: PRP (Properties)
         (bond energy in, NMR in study of)
     ANSWER 71 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     110945-33-0 REGISTRY
RN
     Entered STN: 24 Oct 1987
ED
     Zinc, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
     1-Butanamine, zinc complex
C10 H22 N4 S2 Zn
CN
MF
CI
     CCS
     CA
SR
     STN Files:
                  CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)
            NH2-Bu-n
            2+
  = c = N - Zn - N = C = S
            NH2-Bu-n
                1 REFERENCES IN FILE CA (1907 TO DATE)
                1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
     107:184014 CA
AN
     study of the bond strength in complex compounds by proton NMR
TI
      Galitskaya, S. M.; Pavlenko, L. I.
ΑU
CS
     Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
SO
      CODEN: VLPIAZ; ISSN: 0460-0436
DT
      Journal
      Russian
LA
      65-5 (General Physical Chemistry)
CC
      Section cross-reference(s): 77
     Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN,
AB
     NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in
```

```
he order Z_n > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases
     in the order CN > NCŠ # NCSe.
     bond energy complex NMR; zinc butylamine cyano complex bond energy;
ST
     thiocyanato butylamine cadmium complex bond energy; selenocyanato
     butylamine cadmium complex bond energy; cadmium butylamine cyano complex
     bond energy; mercury butylamine cyano complex bond energy
     Bond energy
IT
         (in Group IIB metal complexes, NMR in study of)
     Nuclear magnetic resonance
IT
         (of Group IIB metal complexes)
                                 32491-88-6... 38255-54-8... 38271-02-2
                   32491-84-2
     32491-81-9
IT
                                    110946-25-3
                                                   110987-94-5
                    110946-24-2
     110945-33-0
     RL: PRP (Properties)
         (bond energy in, NMR in study of)
     ANSWER 72 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     100838-97-9 REGISTRY
RN
     Entered STN: 15 Mar 1986
ED
     Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-0]-, (OC-6-34)- (9CI) (CA INDEX NAME)
CN
     C3 H22 CO N4 O2 S
MF
CI
     CCS
SR
                   CA, CAPLUS
     STN Files:
LC
       CAplus document type: Journal
DT.CA
       Roles from non-patents: FORM (Formation, nonpreparative); PREP
RL.NP
        (Preparation)
      H<sub>3</sub>N
             OH<sub>2</sub>
             3<u>+</u>
Me-NH2
             NH3
      H<sub>3</sub>N
                Me-
```

### REFERENCE 1

104:121904 CA Formation and transformation of amminecarbonatocobalt(III) complexes TI Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R. ΑU Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth. CS Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40 SO CODEN: ZAACAB; ISSN: 0044-2313 Journal DT English LA 78-7 (Inorganic Chemicals and Reactions)
[COCO3(NH3)5]ClO4.H2O, trans-[COCO3(NH3)4(15NH3)]ClO4, and
trans-[COCO3(NH3)4(NH2Me)]ClO4 were prepared The transformation reactions
of these complexes, in which a chelate carbonate ligand is formed and one
NH3 is eliminated, were studied in solution and in the solid state. The CC AB products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific. cobalt ammine carbonate prepn deammoniation; regiochem cobalt ammine ST

```
carbonato deammoniation
     Substitution reaction
IT
         (internal, of cobalt ammine carbonato complexes, regiochem. of)
     Regiochemistry
         (of cobalt ammine carbonato complex internal substitution reactions of)
IT
                      100838-94-6P
     100788-50-9P
IT
     RL: PREP (Preparation)
         (formation by internal substitution reaction of
         tetramminecarbonato(methylamine)cobalt ion and aquation of)
                      100838-95-7P
     100788-51-0P
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation)
         (formation of, by aquation of carbonato complex)
     37549-01-2P
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, by internal substitution reaction of
         pentaamminecarbonatocobalt complex)
                                        100838-99-1P
                      100838-98-0P
     100788-53-2P
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, from carbonato complex in acidified DMF)
                                       100838-97-9P
                      100838-96-8P
     100788-52-1P
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, from carbonato complex in acidified DMSO)
     15244-74-3
IT
     RL: PROC (Process)
         (ion exchange of, with perchlorate)
     91321-36-7
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (mercury ion-catalyzed aquation of)
                     100788-47-4P
     65774-48-3P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (preparation and internal substitution reaction of)
      100788-48-5P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (preparation and reaction of, with carbon dioxide)
      ANSWER 73 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     100838-96-8 REGISTRY
Entered STN: 15 Mar 1986
RN
ED
      Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-0]-,
CN
      (OC-6-43)- (9CI) (CA INDEX NAME)
      C3 H22 Co N4 O2 S
MF
CI
      CCS
      CA
SR
      STN Files:
                    CA, CAPLUS
        CAplus document type:
                                  Journal
DT.CA
        Roles from non-patents: FORM (Formation, nonpreparative); PREP
RL.NP
        (Preparation)
              OH<sub>2</sub>
      H<sub>3</sub>N
Me-NH2-
                  Me-
```

#### REFERENCE 1 Formation and transformation of amminecarbonatocobalt(III) complexes Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R. Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth. Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40 104:121904 CA TI ΑU CS SO CODEN: ZAACAB; ISSN: 0044-2313. Journal DT English 78-7 (Inorganic Chemicals and Reactions) LA CC [CoCo3(NH3)5]clo4.H20, trans-[CoCo3(NH3)4(15NH3)]clo4, and trans-[CoCO3(NH3)4(NH2Me)]Clo4 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. products were identified by 1H NMR spectroscopy. The transformation reactions are not stereospecific. cobalt ammine carbonate prepn deammoniation; regiochem cobalt ammine ST carbonato deammoniation Substitution reaction (internal, of cobalt ammine carbonato complexes, regiochem. of) IT (of cobalt ammine carbonato complex internal substitution reactions of) 100788-50-9P 100838-94-6P IT IT RL: PREP (Preparation) (formation by internal substitution reaction of tetramminecarbonato(methylamine)cobalt ion and aquation of) 100838-95-7P IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, by aquation of carbonato complex) 37549-01-2P IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, by internal substitution reaction of pentaamminecarbonatocobalt complex) 100838-99-1P 100838-98-0P 100788-53-2P IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, from carbonato complex in acidified DMF) 100838-96-8P 100838-97-9P IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, from carbonato complex in acidified DMSO) 15244-74-3 IT RL: PROC (Process) (ion exchange of, with perchlorate) 91321-36-7 IT RL: RCT (Reactant); RACT (Reactant or reagent) (mercury ion-catalyzed aquation of) 65774-48-3P 100788-47-4P IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and internal substitution reaction of) 100788-48-5P IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, with carbon dioxide) ANSWER 74 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9 100788-52-1 REGISTRY Entered STN: 08 Mar 1986 RN

ED

```
Cobalt(3+), triammineaqua(methanamine)[sulfinylbis[methane]-0]-,
CN
      (OC-6-44)- (9CI) (CA INDEX NAME)
MF
      C3 H22 CO N4 O2 S
CI
      CCS
SR
      CA
                      CA, CAPLUS
      STN Files:
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PREP
        (Preparation)
               OH2
      H<sub>3</sub>N
Me-NH2
               NH<sub>3</sub>
       H<sub>3</sub>N
                   Me-
                  1 REFERENCES IN FILE CA (1907 TO DATE)
                  1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      104:121904 CA
AN
      Formation and transformation of amminecarbonatocobalt(III) complexes Balt, S.; De Bolster, M. W. G.; Piriz Mac-Coll, C. R.
TI
ΑU
      Dep. Inorg. Chem., Free Univ., Amsterdam, 1081 HV, Neth.
Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 529, 235-40
CS
SO
      CODEN: ZAACAB; ISSN: 0044-2313
      Journal
DT
      English
LA
      78-7 (Inorganic Chemicals and Reactions)
      [COCO3(NH3)5]Clo4.H20, trans-[COCO3(NH3)4(15NH3)]Clo4, and
      trans-[CoCO3(NH3)4(NH2Me)]Clo4 were prepared The transformation reactions of these complexes, in which a chelate carbonate ligand is formed and one NH3 is eliminated, were studied in solution and in the solid state. The
AB
      products were identified by 1H NMR spectroscopy. The transformation
      reactions are not stereospecific.
      cobalt ammine carbonate prepn deammoniation; regiochem cobalt ammine
ST
      carbonato deammoniation
      Substitution reaction
IT
          (internal, of cobalt ammine carbonato complexes, regiochem. of)
      Regiochemistry
IT
          (of cobalt ammine carbonato complex internal substitution reactions of)
                         100838-94-6P
      100788-50-9P
IT
      RL: PREP (Preparation)
          (formation by internal substitution reaction of
          tetramminecarbonato(methylamine)cobalt ion and aquation of)
                         100838-95-7P
IT
      100788-51-0P
      RL: FORM (Formation, nonpreparative); PREP (Preparation)
          (formation of, by aquation of carbonato complex)
IT
       RL: FORM (Formation, nonpreparative); PREP (Preparation)
```

(formation of, by internal substitution reaction of

RL: FORM (Formation, nonpreparative); PREP (Preparation)

100838-99-1P

pentaamminecarbonatocobalt complex)

100838-98-0P

IT

100788-53-2P

```
(formation of, from carbonato complex in acidified DMF)
                                    100838-97-9P
                     100838-96-8P
     100788-52-1P
IT
     RL: FORM (Formation, nonpreparative); PREP (Preparation)
         (formation of, from carbonato complex in acidified DMSO)
     15244-74-3
IT
     RL: PROC (Process)
         (ion exchange of, with perchlorate)
     91321-36-7
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
(mercury ion-catalyzed aquation of)
                    100788-47-4P
     65774-48-3P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and internal substitution reaction of)
     100788-48-5P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (preparation and reaction of, with carbon dioxide)
     ANSWER 75 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     100681-50-3 REGISTRY
Entered STN: 08 Mar 1986
RN
ED
     Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-0]-, (OC-6-22)-,
CN
     triperchlorate (9CI) (CA INDEX NAME) C7 H31 CO N5 O S . 3 Cl O4
MF
SR
     CA
     STN Files:
                  CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
     CM
           1
          100681-48-9
     CRN
           C7 H31 Co N5 O S
     CMF
     CCI
          CCS
      Me-NH2 NH2-Me
               <del>3+</del> NH2− Me
      Me-NH2 NH2-Me
Me-S
   Me
           2
     CM
     CRN 14797-73-0
     CMF
           cl 04
```

# REFERENCE 1

104:141030 CA  $\Delta N$ syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide, TI dimethylformamide, trimethyl phosphate, and acetonitrile Curtis, Neville J.; Lawrance, Geoffrey A.
Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669 ΑU CS **SO** Journal DT English 78-7 (Inorganic Chemicals and Reactions) CC Section cross-reference(s): 67 Prepns. of [Co(NH2Me)5L]3+ (I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile AΒ and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+(II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. dissociative Id type mechanism operates. The more pos. AS.thermod. and  $\Delta V$ . thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis(methylamine) complexes. These results parallel earlier observations of  $\Delta s$ . thermod. and  $\Delta V$  thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed. cobalt methylamine neutral ligand complex; amine methyl cobalt neutral ST ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation; urea cobalt methylamine aquation Aquation IT Kinetics of aquation (acid, of cobalt methylamine complexes with neutral ligands) Steric effect IT (in acid aquation of cobalt methylamine complexes with neutral ligands) Hydrolysis IT Kinetics of hydrolysis (base, of cobalt acetonitrile methylamine complex) IT RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in acid aquation of cobalt methylamine neutral ligand complexes) 100681-47-8P IT RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and kinetics of acid aquation and base hydrolysis of) 100681-49-0P 100681-50-3P 100681-45-6P 100681-43-4P IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and kinetics of acid aquation of) 90065-88-6 IT RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reactions of, with neutral ligands)

```
ANSWER 76 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
       100681-49-0 REGISTRY
Entered STN: 08 Mar 1986
RN
ED
       Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-0]-, (OC-6-22)-,
CN
       salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
       Methanesulfonic acid, trifluoro-, ion(1-), (OC-6-22)-
pentakis(methanamine)[sulfiny]bis[methane]-0]cobalt(3+) (3:1)
       C7 H31 CO N5 O S . 3 C F3 O3 S
MF
SR
       CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
              1
       CM
       CRN
              100681-48-9
              C7 H31 CO N5 O S
       CMF
       CCI CCS
        Me-NH2 NH2-Me
       Me-NH2 NH2-Me
Me-S
     Мe
              2
       CM
       CRN 37181-39-8
       CMF C F3 03 S
       so3-
                      1 REFERENCES IN FILE CA (1907, TO DATE)
                      1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
       104:141030 CA
ΑN
       syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) complexes of the neutral ligands urea, dimethyl sulfoxide,
TI
       dimethylformamide, trimethyl phosphate, and acetonitrile Curtis, Neville J.; Lawrance, Geoffrey A. Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia Inorganic Chemistry (1986), 25(7), 1033-7 CODEN: INOCAJ; ISSN: 0020-1669
ΑU
CS
S0
DT
        Journal
LA
        English
```

```
78-7 (Inorganic Chemicals and Reactions)
CC
      section cross-reference(s): 67
      Prepns. of [Co(NH2Me)5L]3+(I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile
AB
      and high-yielding. Acid equation reactions of these cations occur with
      rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+ (II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. \Delta S. thermod.
      and AV. thermod. values for I compared with II imply a diminished
      role for an incoming water mol. in the dissociated transition state, which
      accords with the steric crowding known in pentakis (methylamine) complexes.
      These results parallel earlier observations of \Delta S. thermod. and
      AV.thermod. variation in the chloro analogs, although overall
      electrostrictive effects present with the charged leaving group are
      markedly diminished in this case where neutral leaving groups are
      employed.
      cobalt methylamine neutral ligand complex; amine methyl cobalt neutral
ST
      ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt
      methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation;
      urea cobalt methylamine aquation
      Aquation
IT
      Kinetics of aquation
      (acid, of cobalt methylamine complexes with neutral ligands)
Steric effect
IT
           (in acid aquation of cobalt methylamine complexes with neutral ligands)
      Hydrolysis
IT
      Kinetics of hydrolysis
      (base, of cobalt acetonitrile methylamine complex) 32424-84-3P
IT
      RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in acid aquation of cobalt methylamine neutral ligand
          complexes)
      100681-47-8P
IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
           (preparation and kinetics of acid aquation and base hydrolysis of)
                                                                                    100681-52-5P
                                             100681-49-0P
                                                                100681-50-3P
                          100681-45-6P
      100681-43-4P
IT
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
           (preparation and kinetics of acid aquation of)
      90065-88-6
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
           (substitution reactions of, with neutral ligands)
      ANSWER 77 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      100681-48-9 REGISTRY
RN
      Entered STN: 08 Mar 1986
ED
      Cobalt(3+), pentakis(methanamine)[sulfinylbis[methane]-0]-, (OC-6-22)-
CN
       (9CI) (CA INDEX NAME)
      C7 H31 CO N5 O S
MF
CI
      CCS, COM
SR
      CA
```

```
ANSWER 78 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
       100681-45-6 REGISTRY
Entered STN: 08 Mar 1986
RN
       Cobalt(3+), pentakis(methanamine)(trimethyl phosphate-0'')-, (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:3) (9CI) (CA INDEX NAME)
ED
CN
OTHER CA INDEX NAMES:
       Methanesulfonic acid, trifluoro-, ion(1-), (OC-6-22)-
pentakis(methanamine)(trimethyl phosphate-0''')cobalt(3+) (3:1)
Phosphoric acid, trimethyl ester, cobalt complex
C8 H34 Co N5 O4 P . 3 C F3 O3 S
CN
MF
SR
       CA
       STN Files: CA, CAPLUS
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
        CM
        CRN 100681-44-5
        CMF C8 H34 Co N5 O4 P
        CCI CCS
```

# REFERENCE 1

104:141030 CA Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III) TI complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile Curtis, Neville J.; Lawrance, Geoffrey A.
Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia Inorganic Chemistry (1986), 25(7), 1033-7
CODEN: INOCAJ; ISSN: 0020-1669 ΑU CS 50 DT English LA 78-7 (Inorganic Chemicals and Reactions) CC Section cross-reference(s): 67 Prepns. of [Co(NH2Me)5L]3+(I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile AB and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+(II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar, both activation entropies and activation vols. are more pos., yet not particularly sensitive to the size of the neutral leaving group. A dissociative Id type mechanism operates. The more pos. As.thermod. and AV.thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis (methylamine) complexes. These results parallel earlier observations of \( \Delta S. \text{thermod. and} \) ΔV.thermod. variation in the chloro analogs, although overall electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are employed. cobalt methylamine neutral ligand complex; amine methyl cobalt neutral ST ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl cobalt methylamine aquation; acetonitrile cobalt methylamine aquation; urea cobalt methylamine aquation Aquation IT Kinetics of aquation (acid, of cobalt methylamine complexes with neutral ligands) Steric effect IT (in acid aquation of cobalt methylamine complexes with neutral ligands) IT Hydrolysis Kinetics of hydrolysis (base, of cobalt acetonitrile methylamine complex) 32424-84-3P IT RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in acid aquation of cobalt methylamine neutral ligand complexes) 100681-47-8P IT RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and kinetics of acid aquation and base hydrolysis of) 100681-45-6P 100681-49-0P 100681-50-3P 100681-52-5P 100681-43-4P IT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and kinetics of acid aquation of) 90065-88-6 IT RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reactions of, with neutral ligands)

```
ANSWER 79 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     100681-44-5 REGISTRY
Entered STN: 08 Mar 1986
RN
     Cobalt(3+), pentakis(methanamine)(trimethyl phosphate-0''')-, (OC-6-22)-(9CI) (CA INDEX NAME)
ED
CN
OTHER CA INDEX NAMES:
     Phosphoric acid, trimethyl ester, cobalt complex
CN
     C8 H34 Co N5 O4 P
MF
     CCS, COM
CI
SR
     CA
              oMe
               oMe
              ome
Me-NH2
              NH2-Me
         Co 3+
              NH2-Me
Me-NH2
         NH2-Me
     ANSWER 80 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     90065-88-6 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-0)-,
CN
      (OC-6-22)-, salt with trifluoromethanesulfonic acid (1:2) (9CI) (CA INDEX
OTHER CA INDEX NAMES:
     Methanesulfonic acid, trifluoro-, ion(1-), (OC-6-22)-
pentakis(methanamine)(trifluoromethanesulfonato-0)cobalt(2+) (2:1)
      C6 H25 Co F3 N5 O3 S . 2 C F3 O3 S
MF
                   CA, CAPLUS
     STN Files:
LC
DT.CA CAplus document type: Journal
       Roles from non-patents: PREP (Preparation); PRP (Properties); RACT
        (Reactant or reagent)
      CM
           1
      CRN 84254-64-8
      CMF C6 H25 Co F3 N5 O3 S
      CCI CCS
```

CM 2

CRN 37181-39-8 CMF C F3 03 S

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

```
105:107276 CA
 AN
        Pentakis(methanamine)(trifluoromethanesulfonato-0) complexes of
 TI
        chromium(III), cobalt(III), and rhodium(III)
Lawrance, Geoffrey A.; Sargeson, Alan M.
 ΑU
        Dep. Chem., Univ. Newcastle, 2308, Australia Inorganic Syntheses (1986), 24, 279-82 CODEN: INSYA3; ISSN: 0073-8077
 CS
 SO
 DT
        Journal
        English
 LA
        78-7 (Inorganic Chemicals and Reactions)
 CC
        [M(NH2Me)5(OSO2CF3)](SO3CF3)2 (M = Co, Cr, Rh) were prepared from [M(NH2Me)5C1]C12 and CF3SO3H.
 AB
        safety transition metal methylamine trifluoromethanesulfonato 90065-87-5P
 ST
 IT
        RL: SPN (Synthetic preparation); PREP (Preparation)
            (preparation of, from chromium chloro methylamine complex and trifluoromethane sulfonic acid)
 IT
        RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, from cobalt chloro methylamine complex and trifluoromethanesulfonic acid)
 IT
        90065-89-7P
        RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, from rhodium chloro methylamine complex and
             trifluoromethanesulfonic acid)
                                           64459-98-9
                         15392-59-3
. IT
        15351-84-5
        RL: RCT (Reactant); RACT (Reactant or reagent)
```

```
(reaction of, with trifluoromethanesulfonic acid)
```

```
REFERENCE 2
       104:141030 CA
AN
       Syntheses and acid aquation reactions of pentakis(methylamine)cobalt(III)
       complexes of the neutral ligands urea, dimethyl sulfoxide, dimethylformamide, trimethyl phosphate, and acetonitrile Curtis, Neville J.; Lawrance, Geoffrey A.
TI
ΑU
       Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia Inorganic Chemistry (1986), 25(7), 1033-7 CODEN: INOCAJ; ISSN: 0020-1669
CS
S<sub>0</sub>
DT
        Journal
       English
LA
        78-7 (Inorganic Chemicals and Reactions)
CC
        Section cross-reference(s): 67
       Prepns. of [Co(NH2Me)5L]3+(I) cations (L = urea, DMSO, DMF, (MeO)3PO, and CH3CN) based on the [Co(NH2Me)5(OSO2CF3)](CF3SO3)2 precursor are facile
AB
       and high-yielding. Acid equation reactions of these cations occur with rate consts. at least 70-fold faster than those reported for [Co(NH3)5L]3+(II) analogs at 25°, this general rate enhancement being apparently steric in origin. Whereas activation enthalpies for I and II are similar,
       both activation entropies and activation vols. are more pos., yet not
       particularly sensitive to the size of the neutral leaving group.
       dissociative Id type mechanism operates. The more pos. \Delta S. thermod. and \Delta V. thermod. values for I compared with II imply a diminished role for an incoming water mol. in the dissociated transition state, which accords with the steric crowding known in pentakis (methylamine) complexes. These results parallel earlier observations of \Delta S. thermod. and
       ΔV.thermod. variation in the chloro analogs, although overall
        electrostrictive effects present with the charged leaving group are markedly diminished in this case where neutral leaving groups are
        employed.
        cobalt methylamine neutral ligand complex; amine methyl cobalt neutral
ST
        ligand complex; kinetics aquation cobalt methylamine complex; DMSO cobalt
        methylamine aquation; DMF cobalt methylamine aquation; phosphate trimethyl
        cobalt methylamine aquation; acetonitrile cobalt methylamine aquation;
        urea cobalt methylamine aquation
        Aquation
IT
        (acid, of cobalt methylamine complexes with neutral ligands) steric effect
IT
             (in acid aquation of cobalt methylamine complexes with neutral ligands)
        Hydrolysis
IT
        (base, of cobalt acetonitrile methylamine complex)
IT
        RL: FORM (Formation, nonpreparative); PREP (Preparation) (formation of, in acid aquation of cobalt methylamine neutral ligand
             complexes)
        100681-47-8P
IT
        RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and kinetics of acid aquation and base hydrolysis of)
                               100681-45-6P 100681-49-0P 100681-50-3P
                                                                                                      100681-52-5P
        100681-43-4P
IT
        RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
```

```
REFERENCE 3
       101:121855 CA
AN
       Synthetically versatile (trifluoromethanesulfonato)metal amine complexes
TI
       Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan
ΑU
       Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia Inorganic Chemistry (1984), 23(19), 2940-7 CODEN: INOCAJ; ISSN: 0020-1669
CS
S0
DT
       Journal
I A
       English
        78-7 (Inorganic Chemicals and Reactions)
CC
       Section cross-reference(s): 67
       Facile preparation routes to complexes of the labile unidentate coordinated
       Facile preparation routes to complexes of the labile unidentate coordinate -0502CF3 ion are reported for M(NH3)5(0502CF3)n+ (M = Rh, Ir, Cr, Ru, n = 2, M = Pt, n = 3), M(NH2Me)5(0502CF3)2+ (M = Co, Rh, Cr), cis-M(en)2(0502CF3)2+ (M = Rh, Ir, Cr, and trans-M(en)2Cl(0502CF3)+ (M = Rh, Ir). The utility of these synthetically versatile intermediates in the preparation of a variety of complexes containing neutral ligands is illustrated. Rate consts. for the aquation of the triflato complexes in 0.1M CF3503H at 25° span 3 orders of magnitude and for the
AB
        pentaammine complexes show a reactivity order of Ru > Co apprx. Cr
        apprx. Rh » Ir > Pt. For the pentakis(methylamine) complexes, the
        aquation rate is greater for Co, slightly greater for Rh, and smaller for
       Cr in comparison to the corresponding pentaammine complexes.
       aquations of M(en)2X(0S02CF3)+ proceed largely without isomerization (<5%), and the triflato complexes are prepared stereospecifically by this route. For the cis-M(en)2(0S02CF3)2+ ions, consecutive 1st-order aquation processes are observed with rate consts. k1 .apprx. 2k2.
        transition metal amine trifluoromethanesulfonato; aquation kinetics amine
ST
        trifluoromethanesulfonato complex; ammine transition metal
        trifluoromethanesulfonato; methylamine transition metal trifluoromethanesulfonato; ethylenediamine transition metal
        trifluoromethanesulfonato
        Aquation
IT
        Kinetics of aquation
             (of transition metal amine complexes with trifluoromethanesulfonate)
        75522-52-0
IT
        RL: PRP (Properties)
             (kinetics of aquation of)
                                                                                              90065-91-1P
                                                                        90065-89-7P
                             90065-87-5P
                                                   90065-88-6P
        84254-63-7P
IT
        90065-99-9P
        RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and kinetics of aquation of)
                                                                                              87564-83-8P
                                                                         32700-25-7P
                                                   29031-66-1P
        14023-02-0P
                             15611-81-1P
IT
                                                                        90066-05-0P
                                                                                              90084-45-0P
                             90066-03-8P
                                                   90066-04-9P
        90066-01-6P
        90084-46-1P
                             90130-09-9P
        RL: SPN (Synthetic preparation); PREP (Preparation)
             (preparation of)
                             84254-59-1P
        84254-57-9P
IT
        RL: SPN (Synthetic preparation); PREP (Preparation)
```

(preparation, aquation and reaction with ammonia) 84254-61-5P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, aquation and reactions with acetonitrile and urea)

90065-97-7P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, reaction with ammonia and kinetics of aquation of)

IT 90065-95-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, reaction with ethylenediamine and kinetics of aquation of)

IT

```
84278-98-8P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation, reaction with methanol and kinetics of aquation of)
     90065-93-3P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation, reactions with ammonia and ethylenediamine and kinetics of
         aquation of)
                                                                 15392-59-3
                                                  15351-84-5
                    13820-95-6
                                   14240-29-0
     13820-89-8
IT
                                                  15444-63-0
                                                                15742-38-8
                    15444-47-0
                                   15444-62-9
     15444-46-9
                                   64459-98-9
                    18532-87-1
     16893-11-1
     RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with trifluoromethanesulfonic acid)
     ANSWER 81 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     84254-64-8 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Cobalt(2+), pentakis(methanamine)(trifluoromethanesulfonato-0)-, (OC-6-22)- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
     Methanesulfonic acid, trifluoro-, cobalt complex C6 H25 Co F3 N5 O3 S
MF
     CCS, COM
STN Files:
CI
                    CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties); RACT (Reactant or reagent)
```

## REFERENCE 1

NH2-Me

104:96513 CA AN Hydrolysis of coordinated trifluoromethanesulfonate from cobalt(III), TI rhodium(III), iridium(III) and chromium(III) pentaamines
Curtis, Neville J.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan ΑU Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia Inorganic Chemistry (1986), 25(4), 484-8
CODEN: INOCAJ; ISSN: 0020-1669 CS SO DT Journal English 67-3 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms) CC Section cross-reference(s): 78 Base hydrolysis and aquation of M(NH3)5(OSO2CF3)2+ (M = Co, Rh, Ir, Cr) and M(NH2CH3)5(OSO2CF3)2+ (M = Co, Rh, Cr) complexes at 25° and AB

ST

IT

IT

IT

IT

AN

TI

ΑU

CS

SO DT

LA

CC

AB

ST

```
ionic strength 1.0 M are reported. The N-methylation of the ammine ligand causes a marked enhancement of the rate of base hydrolysis reactions with kMe/kH of 2100 (Co), 150 (Rh), and 800 (Cr). Only minor enhancements occur for aquation with Co and Rh, while there is a minor rate diminution with Cr. Pos. activation entropies for base hydrolysis of
        with Cr. Pos. activation entropies for base hydrolysis of M(NH3)5(OSO2CF3)2+ (M = Co, Ir) and competition expts. with azide ion in basic solution as well as the absence of the competing ion in the rate law
         allow a dissociative conjugate-base mechanism for all complexes.
        variation in rate enhancement from ammine to methylamine compds. and the competition studies in base with azide ion chiefly reflect differences in steric interactions due to differing metal-ligand bond lengths rather than any mechanistic diversity. Variations in competition behavior for RhIII), Cr(III), and Co(III) appear to reflect relative lifetimes of the
        cr(III), and Co(III) appear to reflect relative lifetimes of the intermediate of reduced coordination number. The variations in aquation are much smaller and do not allow any certainty in mechanistic assertions. Marked accelerations of rates for both acid and base hydrolyses (.apprx.103-106-fold) occur consistently for all trifluoromethanesulfonato complexes compared with those of halo of analogs. hydrolysis kinetics rhodium 3 fluoromethanesulfonate; cobalt 3 ammine fluoromethanesulfonate hydrolysis; chromium 3 ammine fluoromethanesulfonate hydrolysis.
         hydrolysis; chromium 3 ammine fluoromethanesulfonate hydrolysis
         Transition metals, compounds
         RL: USES (Uses)
                (ammine or amine complexes containing trifluoromethanesulfonate, hydrolysis
               of)
         Aquation
         Hvdrolysis
         Kinetics of aquation
         Kinetics of hydrolysis
               (of transition metal ammine-trifluoromethanesulfonate complexes)
         Ammines
         RL: USES (Uses)
         (transition metal, hydrolysis of trifluoromethanesulfonate ligand from) 75522-49-5 84254-56-8 84254-58-0 84254-60-4 84254-64-8
                                  84254-66-0
         84254-65-9
         RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
                (hydrolysis of, kinetics of)
REFERENCE 2
         98:100163 CA
          (Trifluoromethanesulfonato-0)pentaammine complexes: versatile synthetic
          intermediates
         Dixon, Nicholas E.; Lawrance, Geoffrey A.; Lay, Peter A.; Sargeson, Alan
         Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2600, Australia
         Inorganic Chemistry (1983), 22(5), 846-7 CODEN: INOCAJ; ISSN: 0020-1669
         Journal
          English
          78-7 (Inorganic Chemicals and Reactions)
          Section cross-reference(s): 67
         [M(NH3)5(OSO2CF3)](CF3SO3)n, where M = Cr(III), Rh(III), Ir(III), Ru(III), and Pt(IV), were prepared in essentially quant. yields from the reactions of [M(NH3)5C]]Cln in CF3SO3H. The rate consts. for aquation of [M(NH3)5(OSO2CF3)](CF3SO3)n at 25° (0.1M CF3SO3H) indicate a
         reactivity order of Ru(III) > Rh(III) > Cr(III) > Pt(IV) > Ir(III). Aquation rate consts. for the [M(NH2Me)5(OSO2CF3)]2+ ions (M = Co(III),
         Rh(III), Cr(III)) were determined, and k(NH2Me)/k(NH3) ratios are 4.2, 1.7, and
          0.051 for the Co(III), Rh(III), and Cr(III) complexes, resp.
         ammine trifluoromethanesulfonato transition metal; chromium ammine
```

```
trifluoromethanesulfonato; rhodium ammine trifluoromethanesulfonato;
     iridium ammine trifluoromethanesulfonato; ruthenium ammine
     trifluoromethanesulfonato; platinum ammine trifluoromethanesulfonato;
     aquation kinetics transition metal trifluoromethanesulfonato
     Kinetics of aquation
IT
        (of transition metal trifluoromethanesulfonato complexes)
                  84254-65-9 84254-66-0
     84254-64-8
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (aquation of, kinetics of)
                                  84254-61-5P 84254-63-7P
                                                                84278-98-8P
     84254-57-9P
                  84254-59-1P
IT
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and kinetics of aquation of)
     13820-89-8 13820-95-6 15742-38-8 16893-11-1
                                                           18532-87-1
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (substitution reaction of, with trifluoromethanesulfonic acid)
     ANSWER 82 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
RN
     73358-73-3 REGISTRY
     Entered STN: 16 Nov 1984
     Copper(2+), bis(2-methyl-2-propanamine)tetrakis[sulfinylbis[methane]-0]-
ED
CN
     (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     2-Propanamine, 2-methyl-, copper complex C16 H46 Cu N2 O4 S4
CN
MF
CI
                  CA, CAPLUS
     STN Files:
LC
      CAplus document type: Journal
DT.CA
       Roles from non-patents: FORM (Formation, nonpreparative); PREP
RL.NP
       (Preparation)
```

#### REFERENCE 1

AN 92:153821 CA
Complexing of copper(II) salts with pyridines and primary aliphatic amines in dimethyl sulfoxide
AU Dulova, V. I.; Brezhe, A. L.; Molchanova, N. R.; Artyukhova, E. P. Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
Koordinatsionnaya Khimiya (1980), 6(2), 248-51

```
CODEN: KOKHDC; ISSN: 0132-344X
       Journal
DT
       Russian
LA
      68-2 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
CC
      Section cross-reference(s): 69
      Instability consts. were determined spectrophotometrically and heats of coordination were determined calorimetrically for 1:1 and 1:2 complexes by assuming equilibrium of the type Cu(DMSO)62+ + 2L .dblharw. Cu(DMSO)5L2+ + DMSO; Cu(DMSO)5L2+ + L .dblharw. Cu(DMSO)4L22+ + DMSO. The relative importance of bonding in these complexes is discussed. copper amine complex stability DMSO; pyridine copper amine complex
AB
ST
       stability; thermodn coordination copper pyridine
      Amines, compounds RL: PRP (Properties)
IT
           (copper(II) complexes, in DMSO)
       Entropy
IT
           (of coordination, of copper(II) with amines or pyridines in DMSO)
       Formation constant and Stability constant
IT
           (of copper amine complexes, in DMSO)
       Coordination
IT
       Heat of coordination
           (of copper(II), with amines or pyridines in DMSO)
       Substituent effect
IT
           (on stability, of copper amine and pyridine complexes in DMSO) 58-64-2P 73358-65-3P 73358-66-4P 73358-67-5P 73358-68-
                                                                                   73358-68-6P
IT
       73358-64-2P
                                                                                   73358-73-3P
                                                                73358-72-2P
                          73358-70-0P
                                             73358-71-1P
       73358-69-7P
                          73358-75-5P
                                             73363-32-3P
       73358-74-4P
       RL: FORM (Formation, nonpreparative); PREP (Preparation)
           (formation of, in DMSO)
       ANSWER 83 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
       73358-71-1 REGISTRY
RN
       Entered STN: 16 Nov 1984
ED
       Copper(2+), bis(1-butanamine)tetrakis[sulfinylbis[methane]-0]- (9CI) (CA
CN
       INDEX NAME)
OTHER CA INDEX NAMES:
       1-Butanamine, copper complex C16 H46 Cu N2 O4 S4
CN
MF
CI
       CCS
       STN Files:
                        CA, CAPLUS
LC
        CAplus document type:
                                         Journal
DT.CA
         Roles from non-patents: FORM (Formation, nonpreparative); PREP
RL.NP
          (Preparation)
                     Me
    Me
                      NH2-Bu-n
                      NH2-Bu-n
     Me
                    = S- Me
```

Me

REFERENCE 1

# 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
92:153821 CA
AN
     Complexing of copper(II) salts with pyridines and primary aliphatic amines
TI
      in dimethyl sulfoxide
     Dulova, V. I.; Brezhe, A. L.; Molchanova, N. R.; Artyukhova, E. P. Dnepropetr. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR Koordinatsionnaya Khimiya (1980), 6(2), 248-51
ΑU
CS
SO.
      CODEN: KOKHDC; ISSN: 0132-344X
DT
      Journal
      Russian
LA
      68-2 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
CC
      Section cross-reference(s): 69
      Instability consts. were determined spectrophotometrically and heats of
AΒ
      coordination were determined calorimetrically for 1:1 and 1:2 complexes by assuming equilibrium of the type Cu(DMSO)62+ + 2L .dblharw. Cu(DMSO)5L2+ +
      DMSO; Cu(DMSO)5L2+ + L .dblharw. Cu(DMSO)4L22+ + DMSO. The relative importance of bonding in these complexes is discussed.
      copper amine complex stability DMSO; pyridine copper amine complex
ST
      stability; thermodn coordination copper pyridine
      Amines, compounds RL: PRP (Properties)
IT
          (copper(II) complexes, in DMSO)
      Entropy
ΙT
          (of coordination, of copper(II) with amines or pyridines in DMSO)
      Formation constant and Stability constant
IT
          (of copper amine complexes, in DMSO)
      Coordination
IT
      Heat of coordination
          (of copper(II), with amines or pyridines in DMSO)
      Substituent effect
IT
          (on stability, of copper amine and pyridine complexes in DMSO) 58-64-2P 73358-65-3P 73358-66-4P 73358-67-5P 73358-68-
                                                                           73358-68-6P
IT
      73358-64-2P
                                                          73358-72-2P
                                                                           73358-73-3P
                                        73358-71-1P
                       73358-70-0P
      73358-69-7P
                       73358-75-5P
                                        73363-32-3P
      73358-74-4P
      RL: FORM (Formation, nonpreparative); PREP (Preparation)
          (formation of, in DMSO)
      ANSWER 84 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      67008-65-5 REGISTRY
RN
      Entered STN: 16 Nov 1984
Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-
ED
CN
      N,N',O,O']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-
      butanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9C1) (CA INDEX NAME)
OTHER CA INDEX NAMES:
      1-Butanamine, cobalt complex
      1-Propanamine, cobalt complex
CN
      2-Pentanone, 4,4'-(1,2-ethanediyldinitrilo)bis-, cobalt complex Cobaltate(1-), bis(1-butanamine)tetrakis(thiocyanato-N)-, (OC-6-11)-,
CN
CN
      (OC-6-22)-[[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-
      N,N',0,0']bis(1-propanamine)cobalt(1+) (9CI)
      C18 H36 CO N4 O2 . C12 H22 CO N6 S4 STN Files: CA, CAPLUS
MF
DT.CA CAplus document type:
                                    Journal
RL.NP Roles from non-patents: PREP (Preparation)
```

Ring System Data

# Page 236

Elemental	Elemental	Size of	Ring System	Ring	RID
Analysis	Sequence	the Rings	Formula	Identifier	Occurrence
EA	ES	SZ	RF	RID	Count
======================================	CONCENT	, , , ,	C8CoN2O2 	1620.11.3	1 in CM  2

CM 1

CRN 66915-23-9 CMF C12 H22 CO N6 S4 CCI CCS

$$S = C = N^{-}$$
 $N = C = S$ 
 $N = C = S$ 

CM 2

CRN 30649-39-9 CMF C18 H36 CO N4 O2 CCI CCS

PAGE 1-A

R2 \ NH2-- Pr-n

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

```
89:52589 CA
      New tetrathiocyanatodiaminechromates with aliphatic monoamines
TI
      Ganescu, I.; Varhelyi, C.; Futo, F.; Brinzan, G.
ΑU
      Chem. Fak., Univ. Craiova, Craiova, Rom.
Zeitschrift fuer Anorganische und Allgemeine Chemie (1978), 439, 282-8
CS
SO
      CODEN: ZAACAB; ISSN: 0044-2313
      Journal
DT
      German
LA
      78-7 (Inorganic Chemicals and Reactions)
CC
      [Cr(NCs)4L2]- (L = PrNH2, BuNH2) were prepared by a substitution reaction of K3[Cr(NCs)6] with L in the molten state. Twenty_complex salts of the type
AB
      R.H[Cr(NCS)4L2] (L = amine) and 20 Co-amine complexes with [Co(NCS)4L2]-were isolated. The complexes were characterized by IR and UV spectra.
      cobalt amine thiocyanato; propylamine cobalt thiocyanato; butylamine
ST
      cobalt thiocyanato
                                           66915-21-7P
66915-28-4P
66915-34-2P
                                                              66915-24-0P
                                                                                66915-25-1P
                         66915-20-6P
      66915-18-2P
IT
                                                              66915-29-5P
                                                                                66915-30-8P
                         66915-27-3P
      66915-26-2P
                                                              66915-35-3P
                                                                                66915-36-4P
                         66915-33-1P
      66915-32-0P
                                                              66915-41-1P
                                                                                 66915-42-2P
                                           66915-39-7P
                         66915-38-6P
      66915-37-5P
                                                                                 66915-47-7P
                                           66915-45-5P
                                                              66915-46-6P
                         66915-44-4P
      66915-43-3P
                                                                                 67008-64-4P
                                                              66969-93-5P
                                           66969-92-4P
                         66969-90-2P
      66964-00-9P
                                                                                67008-69-9P
                                           67008-67-7P
                                                              67008-68-8P
                         67008-66-6P
      67008-65-5P
                                                                                67146-76-3P
                                                              67146-75-2P
                                           67146-74-1P
      67008-70-2P
                         67008-71-3P
      RL: SPN (Synthetic preparation); PREP (Preparation)
           (preparation of)
      ANSWER 85 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
RN
      67008-64-4 REGISTRY
      Entered STN: 16 Nov 1984
ED
      Cobalt(1+), [[4,4'-(1,2-ethanediyldinitrilo)bis[2-pentanonato]](2-)-N,N',0,0']bis(1-propanamine)-, (OC-6-22)-, (OC-6-11)-bis(1-propanamine)tetrakis(thiocyanato-N)cobaltate(1-) (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
      1-Propanamine, cobalt complex 2-Pentanone, 4,4'-(1,2-ethanediyldinitrilo)bis-, cobalt complex
CN
CN
      Cobaltate(1-), bis(1-propanamine)tetrakis(thiocyanato-N)-, (OC-6-11)-, (OC-6-22)-[[4,4'-(1,2-ethanediy)]dinitrilo)bis[2-pentanonato]](2-)-
CN
      N,N',O,O']bis(1-propanamine)cobalt(1+) (9CI)
      C18 H36 CO N4 O2 . C10 H18 CO N6 S4
MF
                       CA, CAPLUS
      STN Files:
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation)
Ring System Data
```

| Size of |Ring System|

RF

|the Rings|

SZ

Elemental

Sequence

ES

Ring

RID

Formula | Identifier | Occurrence

| Count

Elemental

Analysis

EΑ

# Page 238

C2CoN2- | CONC2N- | 5-6-6 | C8CoN2O2 | 1620.11.3 | 1 in CM | C3CoNO-C3CONO | CONC3O-CONC3O | CONC3O-CONC3O-CONC3O | CONC3O-CONC3O

CM 1

CRN 66915-22-8 CMF C10 H18 CO N6 S4 CCI CCS

 $S = C = N - \begin{vmatrix} N = C = S \\ N = C = S \end{vmatrix}$  N = C = S N = C = S N = C = S N = C = S N = C = S

CM 2

CRN 30649-39-9 CMF C18 H36 CO N4 O2 CCI CCS

PAGE 1-A

PAGE 2-A

## REFERENCE 1

```
89:52589 CA
AN
      New tetrathiocyanatodiaminechromates with aliphatic monoamines
      Ganescu, I.; Varhelyi, C.; Futo, F.; Brinzan, G.
Chem. Fak., Univ. Craiova, Craiova, Rom.
Zeitschrift fuer Anorganische und Allgemeine Chemie (1978), 439, 282-8
TI
ΑU
CS
S0
      CODEN: ZAACAB; ISSN: 0044-2313
      Journal
DT
      German
LA
      78-7 (Inorganic Chemicals and Reactions)
CC
      [Cr(NCS)4L2]- (L = PrNH2, BuNH2) were prepared by a substitution reaction of
AΒ
      K3[Cr(NCS)6] with L in the molten state. Twenty complex salts of the type R.H[Cr(NCS)4L2] (L = amine) and 20 Co-amine complexes with [Co(NCS)4L2]-were isolated. The complexes were characterized by IR and UV spectra. cobalt amine thiocyanato; propylamine cobalt thiocyanato; butylamine
ST
      cobalt thiocyanato
                                                                                66915-25-1P
                                           66915-21-7P
                                                             66915-24-0P
      66915-18-2P
66915-26-2P
                         66915-20-6P
IT
                                                                                66915-30-8P
                                                             66915-29-5P
                         66915-27-3P
                                           66915-28-4P
                                                              66915-35-3P
                                                                                66915-36-4P
                         66915-33-1P
      66915-32-0P
                                           66915-34-2P
                                                                                66915-42-2P
                                           66915-39-7P
                                                             66915-41-1P
                         66915-38-6P
      66915-37-5P
                                                                                66915-47-7P
      66915-43-3P
                                           66915-45-5P
                                                             66915-46-6P
                         66915-44-4P
                                                                                67008-64-4P
                                                             66969-93-5P
                                           66969-92-4P
      66964-00-9P
                         66969-90-2P
                                                                                67008-69-9P
                                           67008-67-7P
                                                              67008-68-8P
                         67008-66-6P
      67008-65-5P
                                                                                67146-76-3P
                                                              67146-75-2P
                         67008-71-3P
                                           67146-74-1P
      67008-70-2P
      RL: SPN (Synthetic preparation); PREP (Preparation)
           (preparation of)
      ANSWER 86 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
      66915-23-9 REGISTRY
RN
      Entered STN: 16 Nov 1984 Cobaltate(1-), bis(1-butanamine)tetrakis(thiocyanato-N)-, (OC-6-11)- (9CI)
ED
CN
       (CA INDEX NAME)
OTHER CA INDEX NAMES:
      1-Butanamine, cobalt complex
CN
      C12 H22 CO N6 S4
MF
CI
      CCS, COM
```

$$S = C = N$$
 $N = C = S$ 
 $N = C = S$ 

```
L9 ANSWER 87 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 66915-22-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cobaltate(1-), bis(1-propanamine)tetrakis(thiocyanato-N)-, (OC-6-11)-
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
```

## Page 240

CN 1-propanamine, cobalt complex MF C10 H18 Co N6 S4 CI CCS, COM

$$S = C = N^{-}$$
 $N = C = S$ 
 $N = C = S$ 

ANSWER 88 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN L9 61914-81-6 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, tetrakis(methanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA CN INDEX NAME) C6 H20 N6 Ni S2 MF CI CCS STN Files: CA, CAPLUS LC DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

Me-NH2 NH2-Me

Me-NH2-Ni
$$\frac{2+}{-}$$
N=C-S

Me-NH2 N=C-S

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

86:83070 CA AN Heterogeneous reactions of solid nickel(II) complexes. X. Study of TI stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines Jona, E.; Vojtas, B.; Sramko, T. Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 107-13 CODEN: CHZVAN; ISSN: 0366-6352 ΑU CS SO Journal DT English LA 78-9 (Inorganic Chemicals and Reactions)
Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol.
NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et;
pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep CC AB decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra.

```
nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine
ST
      thermal decompn
      X-ray
IT
           (diffraction of, by nickel isothiocyanato metal amine complex thermal
          decomposition products)
                         61896-86-4P
      61896-84-2P
      RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and thermal decomposition of)
IT
                         61896-82-0P
      61896-80-8P
IT
      RL: PREP (Preparation)
           (formation, x-ray diffraction and thermal decomposition of)
                      61876-10-6 61896-88-6 61914-81-6
      55091-16-2
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
           (thermal decomposition of)
REFERENCE 2
AN
      86:83011 CA
      Isomerism of nickel(II) complexes. VIII. Study of isomerism of isothiocyanatonickel(II) complexes with some alkylamines
TI
      Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J.
Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
Journal
ΑU
CS
SO
DT
       English
LA
       78-7 (Inorganic Chemicals and Reactions)
      Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed
CC
       at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2Me)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the
       monomer isomerizes to the green pseudooctahedral polymer. Steric effects in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic
       spectra.
       nickel isothiocyanato amine complex isomerism; steric effect nickel
ST
       isothiocyanato amine; thiocyanato nickel amine complex
       Isomerism and Isomers
IT
           (of nickel isothiocyanato alkylamine complexes)
                                                                                 61896-88-6P
                                            61896-84-2P
                                                               61896-86-4P
                         61876-10-6P
       55091-16-2P
IT
       61914-81-6P
       RL: SPN (Synthetic preparation); PREP (Preparation)
           (preparation of)
       ANSWER 89 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
RN
       61896-86-4 REGISTRY
       Entered STN: 16 Nov 1984
ED
       Nickel, bis(ethanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
CN
OTHER CA INDEX NAMES:
       Ethanamine, nickel complex, homopolymer
CN
MF
       (C6 H14 N4 Ni S2)x
CI
                        CA, CAPLUS
       STN Files:
LC
DT.CA CAplus document type:
                                        Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)
              1
       CM
       CRN 61896-85-3
```

CMF C6 H14 N4 Ni S2 CCI CCS

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

86:83070 CA AN Heterogeneous reactions of solid nickel(II) complexes. X. Study of TI stoichiometry of thermal decomposition of isothiocyanatonickel(II)

complexes with some alkylamines

Jona, E.; Vojtas, B.; Sramko, T. Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 107-13 CODEN: CHZVAN; ISSN: 0366-6352 ΑU CS

SO

Journal DT

English LA

78-9 (Inorganic Chemicals and Reactions) CC

Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem, changes in the coordination polyhedra. AB stereochem. changes in the coordination polyhedra.

nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine thermal decompn ST

IT (diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)

61896-84-2P 61896-86-4P IT

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (formation and thermal decomposition of)

61896-82-0P 61896-80-8P IT

RL: PREP (Preparation)

(formation, x-ray diffraction and thermal decomposition of) 91-16-2 61876-10-6 61896-88-6 61914-81-6 55091-16-2 IT RL: RCT (Reactant); RACT (Reactant or reagent)

(thermal decomposition of)

### REFERENCE 2

86:83011 CA AN Isomerism of nickel(II) complexes. VIII. Study of isomerism of isothiocyanatonickel(II) complexes with some alkylamines TI

ΑU

CS

Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J. Dep. Inorg. Chem., slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 100-6 SO

CODEN: CHZVAN; ISSN: 0366-6352

DT Journal English LA

78-7 (Inorganic Chemicals and Reactions) CC Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave AB pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed pseudooctaneural NI(NCS)2(NH2ME)4 and NI(NCS)2(NH2EL)4 which were decomposed at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2ME)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the monomer isomerizes to the green pseudooctahedral polymer. Steric effects in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic nickel isothiocyanato amine complex isomerism; steric effect nickel ST isothiocyanato amine; thiocyanato nickel amine complex Isomerism and Isomers
(of nickel isothiocyanato alkylamine complexes) IT 61896-88-6P 61896-84-2P 61896-86-4P 61876-10-6P 55091-16-2P IT 61914-81-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) ANSWER 90 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9 61896-85-3 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, bis(ethanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME) CN OTHER CA INDEX NAMES: Ethanamine, nickel complex C6 H14 N4 Ni S2 CN MF CCS, COM CI

ANSWER 91 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN L9 61896-84-2 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX CN (C4 H10 N4 Ni S2)x MF **PMS** CI STN Files: CA, CAPLUS DT.CA CAplus document type: Journal Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent) RL.NP 1 CM 61896-83-1 CRN C4 H10 N4 Ni S2 CMF CCI CCS

### REFERENCE 1

- 86:83070 CA ΑN Heterogeneous reactions of solid nickel(II) complexes. X. TI stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines
- ΑU
- Jona, E.; Vojtas, B.; Sramko, T. Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 107-13 CS
- SO CODEN: CHZVAN; ISSN: 0366-6352
- Journal DT
- English LA
- 78-9 (Inorganic Chemicals and Reactions) CC
- Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to AΒ stereochem. changes in the coordination polyhedra.
  nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine
  thermal decompn
- ST
- X-ray IT (diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products)
- 61896-86-4P IT
  - RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (formation and thermal decomposition of)
- 61896-82-0P 61896-80-8P IT
  - RL: PREP (Preparation) (formation, x-ray diffraction and thermal decomposition of) 91-16-2 61876-10-6 61896-88-6 61914-81-6
- IT RL: RCT (Reactant); RACT (Reactant or reagent) (thermal decomposition of)

# REFERENCE 2

- 86:83011 CA AN Isomerism of nickel(II) complexes. VIII. Study of isomerism of TI isothiocyanatonickel(II) complexes with some alkylamines
- ΑU
- CS
- Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J. Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 100-6
  CODEN: CHZVAN; ISSN: 0366-6352 S0
- Journal DT
- English LA
- 78-7 (Inorganic Chemicals and Reactions) CC
- Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed at 130 and 110° magnetic and AB at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2Me)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the monomer isomerizes to the green pseudooctahedral polymer. Steric effects in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic spectra.
- nickel isothiocyanato amine complex isomerism; steric effect nickel ST isothiocyanato amine; thiocyanato nickel amine complex

```
Page 245
      Isomerism and Isomers
          (of nickel isothiocyanato alkylamine complexes)
 IT
                                                    61896-86-4P
                                                                    61896-88-6P
                      61876-10-6P
                                     61896-84-2P
       55091-16-2P
 IT
       61914-81-6P
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (preparation of)
      ANSWER 92 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
 L9
      61896-83-1 REGISTRY
 RN
      Entered STN: 16 Nov 1984
 ED
      Nickel, bis(methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
 CN
      C4 H10 N4 Ni S2
 MF
      CCS, COM
 CI
            NH2-Me
            NH2-Me
      ANSWER 93 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
 L9
       61896-82-0 REGISTRY
 RN
       Entered STN: 16 Nov 1984
 ED
       Nickel, (methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
 CN
       NAME)
       (C3 H5 N3 Ni S2)x
 MF
       PMS
 CI
       STN Files:
                   CA, CAPLUS
 LC
 DT.CA CAplus document type: Journal
  RL.NP Roles from non-patents: PREP (Preparation)
       CM
            1
       CRN 61896-81-9
           C3 H5 N3 Ni S2
       CMF
       CCI CCS
         2+
  NC---- S--
                  1 REFERENCES IN FILE CA. (1907 TO DATE)
                  1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
  REFERENCE 1
       86:83070 CA
  AN
       Heterogeneous reactions of solid nickel(II) complexes. X. Study of
  TI
       stoichiometry of thermal decomposition of isothiocyanatonickel(II)
       complexes with some alkylamines
       Jona, E.; Vojtas, B.; Sramko, T.
Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
Chemicke Zvesti (1976), 30(1), 107-13
CODEN: CHZVAN; ISSN: 0366-6352
  ΑU
  CS
  SO
  DT
       Journal
```

English

LA

Æ

```
78-9 (Inorganic Chemicals and Reactions)
CC
     Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et;
     pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss
     of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the
     decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to
     stereochem. changes in the coordination polyhedra.
     nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine
ST
     thermal decompn
IT
     X-ray
         (diffraction of, by nickel isothiocyanato metal amine complex thermal
         decomposition products)
                   61896-86-4P
     61896-84-2P
IT
     RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (formation and thermal decomposition of)
     61896-80-8P
                   61896-82-0P
IT
     RL: PREP (Preparation)
         (formation, x-ray diffraction and thermal decomposition of)
                                                  61914-81-6
                    61876-10-6 61896-88-6
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (thermal decomposition of)
     ANSWER 94 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     61896-81-9 REGISTRY
RN
     Entered STN: 16 Nov 1984
     Nickel, (methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME) C3 H5 N3 Ni S2
ED
CN
MF
CI
     CCS, COM
           NH2-Me
        2+ |
          - N1 - S - CN
     ANSWER 95 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      61896-80-8 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
     Nickel, tris(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
CN
      NAME)
      (C5 H15 N5 Ni S2)x
MF
CI
      PMS
                    CA, CAPLUS
     STN Files:
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
      CM
           1
           61896-79-5
           C5 H15 N5 Ni S2
      CMF
           CCS
      CCI
```

1 REFERENCES IN FILE CA (1907 TO DATE)

### REFERENCE 1

86:83070 CA AN Heterogeneous reactions of solid nickel(II) complexes. X. Study of TI stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines Jona, E.; Vojtas, B.; Sramko, T. Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 107-13 CODEN: CHZVAN; ISSN: 0366-6352 ΑU CS SO Journal DT English LA 78-9 (Inorganic Chemicals and Reactions) CC Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol. NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et; AB pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the decomposition of I by x-ray diffraction and IR spectra. The multistep decompns. of I and II are related to their crystal structures and not to stereochem. changes in the coordination polyhedra. nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine ST thermal decompn IT X-ray (diffraction of, by nickel isothiocyanato metal amine complex thermal decomposition products) 61896-86-4P 61896-84-2P IT RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (formation and thermal decomposition of) 61896-82-0P 61896-80-8P IT RL: PREP (Preparation) (formation, x-ray diffraction and thermal decomposition of) 55091-16-2 61876-10-6 61896-88-6 61914-8 RL: RCT (Reactant); RACT (Reactant or reagent) 61914-81-6 IT (thermal decomposition of) ANSWER 96 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN L9 61896-79-5 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, tris(methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME) CN C5 H15 N5 Ni S2 MF CCS, COM CI

ANSWER 97 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9 61876-10-6 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, tetrakis(ethanamine)bis(thiocyanato-N)-, (OC-6-12)- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES: Ethanamine, nickel complex C10 H28 N6 Ni S2 MF CI CCS CA, CAPLUS STN Files: DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

86:83070 CA AN Heterogeneous reactions of solid nickel(II) complexes. X. Study of TI stoichiometry of thermal decomposition of isothiocyanatonickel(II) complexes with some alkylamines Jona, E.; Vojtas, B.; Sramko, T. Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech. Chemicke Zvesti (1976), 30(1), 107-13 CODEN: CHZVAN; ISSN: 0366-6352 ΑU CS DΤ Journal English LA /8-9 (Inorganic Chemicals and Reactions)
Ni(NCS)2(NH2Me)4 (I) decomps. in 3 steps, with loss of 2, 1, and 1 mol.
NH2Me; Ni(NCS)2(NH2Et)4 (II) in 2 steps, with loss of 2 and 2 mol. NH2Et;
pseudooctahedral and square-planar Ni(NCS)2(NHEt2)2 in 1 step, with loss
of 2 mol. NHEt2. An intermediate, Ni(NCS)2(NH2Me)3, is indicated in the
decomposition of I by x-ray diffraction and IR spectra. The multistep
decompns. of I and II are related to their crystal structures and not to
stereochem. changes in the coordination polyhedra.
nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine 78-9 (Inorganic Chemicals and Reactions) CC AB nickel isothiocyanato amine thermal decompn; thiocyanato nickel amine ST

```
thermal decompn
      X-ray
IT
          diffraction of, by nickel isothiocyanato metal amine complex thermal
          decomposition products)
                       61896-86-4P
      61896-84-2P
IT
      RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
          (formation and thermal decomposition of)
                       61896-82-0P
      61896-80-8P
IT
      RL: PREP (Preparation)
          (formation, x-ray diffraction and thermal decomposition of)
                    61876-10-6 61896-88-6 61914-81-6
      55091-16-2
IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (thermal decomposition of)
REFERENCE 2
      86:83011 CA
      Isomerism of nickel(II) complexes. VIII. Study of isomerism of
ΤI
      isothiocyanatonickel(II) complexes with some alkylamines
      Jona, E.; Vojtas, B.; Sramko, T.; Gazo, J.
Dep. Inorg. Chem., Slovak Tech. Univ., Bratislava, Czech.
Chemicke Zvesti (1976), 30(1), 100-6
CODEN: CHZVAN; ISSN: 0366-6352
ΑU
CS
SO
DT
      Journal
      English
LA
      78-7 (Inorganic Chemicals and Reactions)
CC
      Exposing Ni(NCS)2 for 2 days to vapors of the appropriate amine gave
      pseudooctahedral Ni(NCS)2(NH2Me)4 and Ni(NCS)2(NH2Et)4 which were decomposed
      at 130 and 110°, resp. to polymeric Ni(NCS)2(NH2Me)2 and Ni(NCS)2(NH2Et)2. The square-planar red isomer of Ni(NCS)2(NHEt2)2 were prepared by reaction of Ni(NCS)2 with liquid Et2NH; in contact with air the monomer isomerizes to the green pseudooctahedral polymer. Steric effects
      in the formation of these complexes are discussed. The complexes were characterized by chemical anal., magnetic moments, and IR and electronic
      nickel isothiocyanato amine complex isomerism; steric effect nickel
ST
      isothiocyanato amine; thiocyanato nickel amine complex
      Isomerism and Isomers
IT
          (of nickel isothiocyanato alkylamine complexes)
                                                                           61896-88-6P
                                                          61896-86-4P
                                        61896-84-2P
      55091-16-2P
                       61876-10-6P
IT
      61914-81-6P
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (preparation of)
      ANSWER 98 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
      60865-94-3 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
      Copper, bis(methanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
CN
      NAME)
      (C4 H10 Cu N4 S2)x
MF
CI
      PMS
                      CA, CAPLUS
      STN Files:
DT.CA CAplus document type: Conference
RL.NP Roles from non-patents: PREP (Preparation)
      CM
            1
            60865-93-2
      CRN
            C4 H10 Cu N4 S2
      CMF
      CCI
```

### REFERENCE 1

```
85:171027 CA Copper(II) aminothiocyanates and aminoselenocyanates
AN
TI
        Skopenko, V. V.; Savitskii, V. N.
ΑU
        Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg.
         Kiev. Gos. Univ., Kiev, USSR
S0
        Khim., Novosibirsk, USSR. CODEN: 34BFAN
DT
         conference
        Russian 78-7 (Inorganic Chemicals and Reactions) Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment. copper amine selenocvanate thiocvanate: bipyridine copper selenocvanate
LA
CC
AB
         copper amine selenocyanate thiocyanate; bipyridine copper selenocyanate
ST
         thiocyanate; phenanthroline copper selenocyanate thiocyanate;
         ethylenediamine copper selenocyanate thiocyanate; butylamine copper
         selenocyanate thiocyanate; methylamine copper selenocyanate thiocyanate;
         propylamine copper selenocyanate thiocyanate 19652-73-4P 22937-31-1P 60865-90-9P 608
                                                                                                               60865-94-3P
                                                                                     60865-92-1P
IT
                                                                                                               60869-54-7P
                                                                                     60866-01-5P
60869-58-1P
                                                            60865-99-8P
                                  60865-98-7P
         60865-96-5P
                                                            60869-57-0P
                                  60869-56-9P
         60869-55-8P
         RL: SPN (Synthetic preparation); PREP (Preparation)
               (preparation of)
         ANSWER 99 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
         60865-93-2 REGISTRY
RN
         Entered STN: 16 Nov 1984
ED
         Copper, bis(methanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
CN
         C4 H10 Cu N4 S2
MF
```

CCS, COM

L9 ANSWER 100 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN

CI

```
60865-92-1 REGISTRY
RN
       Entered STN: 16 Nov 1984
Copper, bis(1-butanamine)bis(thiocyanato-S)-, homopolymer (9CI) (CA INDEX
ED
CN
OTHER CA INDEX NAMES:
       1-Butanamine, copper complex, homopolymer (C10 H22 Cu N4 S2)x
CN
MF
CI
       STN Files:
                            CA, CAPLUS
LC
DT.CA CAplus document type: Conference
RL.NP Roles from non-patents: PREP (Preparation)
       CM
                1
       CRN
               60865-91-0
               C10 H22 Cu N4 S2
       CMF
        CCI
              CCS
                              - CN
                          Cu-NH2-Bu-n
n-Bu-NH2-
                          S-CN
                        1 REFERENCES IN FILE CA (1907 TO DATE)
                        1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
        85:171027 CA
AN
        Copper(II) aminothiocyanates and aminoselenocyanates
TI
        Skopenko, V. V.; Savitskii, V. N.
ΑU
        Kiev. Gos. Univ., Kiev, USSR
CS
        Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg.
SO
        Khim., Novosibirsk, USSR. CODEN: 34BFAN
        conference
DT
        Russian
LA
       Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal
        78-7 (Inorganic Chemicals and Reactions)
CC
AB
        XCN groups are bridging. The Cu atom in Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment.
        copper amine selenocyanate thiocyanate; bipyridine copper selenocyanate
ST
        thiocyanate; phenanthroline copper selenocyanate thiocyanate; ethylenediamine copper selenocyanate thiocyanate; butylamine copper selenocyanate thiocyanate;
        selenocyanate thiocyanate; methylamine copper selenocyanate thiocyanate;
        propylamine copper selenocyanate thiocyanate 19652-73-4P 22937-31-1P 60865-90-9P 608
                                                                           60865-92-1P
                                                                                                 60865-94-3P
                              22937-31-1P
        19652-73-4P
IT
                                                                           60866-01-5P
                                                     60865-99-8P
                                                                                                 60869-54-7P
                              60865-98-7P
        60865-96-5P
                                                                           60869-58-1P
                                                     60869-57-0P
                              60869-56-9P
        60869-55-8P
        RL: SPN (Synthetic preparation); PREP (Preparation)
```

## (preparation of)

L9 ANSWER 101 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 60865-91-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Copper, bis(1-butanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Butanamine, copper complex
MF C10 H22 Cu N4 S2
CI CCS, COM

ANSWER 102 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9 60865-90-9 REGISTRY RN Entered STN: 16 Nov 1984 ED Copper, bis(1-propanamine)bis(thiocyanato-S)-, homopolymer (9CI) CN INDEX NAME) OTHER CA INDEX NAMES: 1-Propanamine, copper complex, homopolymer (C8 H18 Cu N4 S2)x MF CI **PMS** STN Files: CA, CAPLUS LC DT.CA CAplus document type: Conference RL.NP Roles from non-patents: PREP (Preparation) CM 1

CRN 60865-89-6 CMF C8 H18 Cu N4 S2 CCI CCS

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

AN 85:171027 CA
TI Copper(II) aminothiocyanates and aminoselenocyanates
AU Skopenko, V. V.; Savitskii, V. N.
CS Kiev. Gos. Univ., Kiev, USSR
Tezisy Dokl. - Vses. Chugaevskoe Soveshch. Khim. Kompleksn. Soedin., 12th (1975), Volume 3, 421 Publisher: Akad. Nauk SSSR, Sib. Otd., Inst. Neorg. Khim., Novosibirsk, USSR.

```
CODEN: 34BFAN
DT
       conference
       Russian
LA
       78-7 (Inorganic Chemicals and Reactions)
      Cu(RNH2)2(NCS)2 (R = Pr, Bu), Cu(MeNH2)2(NCX)2 (X = S, Se), Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), Cu(bipy)2(NCX)2, and Cuen2(NCSe)Z (Z = Cl, Br, NCS, NO3) were prepared and characterized by ir, EPR, and electronic spectra and magnetic characterized by \frac{1}{2} Cu(NNH2)2(NCS)2.
CC
AB
       measurements. In Cu(RNH2)2(NCS)2, Cu(MeNH2)2(NCX)2, and CuL(NCX)2 (L = bipy, phen), the Cu atom has a square bipyramidal configuration and the
      XCN groups are bridging. The Cu-atom in-Cu(bipy)2(NCX)2 has a trigonal bipyramidal configuration. The NCX groups are N-bonded. The Cu atom in Cuen2(NCSe)Z has a square bipyramidal environment.
       copper amine selenocyanate thiocyanate; bipyridine copper selenocyanate
ST
       thiocyanate; phenanthroline copper selenocyanate thiocyanate;
       ethylenediamine copper selenocyanate thiocyanate; butylamine copper
       selenocyanate thiocyanate; methylamine copper selenocyanate thiocyanate;
       propylamine copper selenocyanate thiocyanate
                                                                   60865-92-1P
                                                                                      .60865-94-3P
                           22937-31-1P
                                               60865-90-9P
       19652-73-4P
IT
                                                                   60866-01-5P
                                                                                       60869-54-7P
                                               60865-99-8P
                           60865-98-7P
       60865-96-5P
                                                                   60869-58-1P
                                               60869-57-0P
                           60869-56-9P
       60869-55-8P
       RL: SPN (Synthetic preparation); PREP (Preparation)
            (preparation of)
       ANSWER 103 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
       60865-89-6 REGISTRY
RN
       Entered STN: 16 Nov 1984
ED
       Copper, bis(1-propanamine)bis(thiocyanato-S)- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
       1-Propanamine, copper complex C8 H18 Cu N4 S2
CN
MF
       CCS, COM
CI
n-Pr-NH2-
```

```
ANSWER 104 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     59710-34-8 REGISTRY
RN
     Entered STN: 16 Nov 1984
CN Cobalt, bis(4-amino-N-2-thiazolylbenzenesulfonamidato-NN)bis(2-methyl-1-propanamine)-, (T-4)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:
     1-Propanamine, 2-methyl-, cobalt complex
CN
     Benzenesulfonamide, 4-amino-N-2-thiazolyl-, cobalt complex
CN
     C26 H38 CO N8 O4 S4
MF
     CCS
CI
     STN Files:
                   CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                  Rina
Analysis | Sequence | the Rings | Formula | Identifier | Occurrence
```

EA	ES	SZ	RF	RID	Count ==+=======
======== C3NS C6	+======   NCSC2   C6	==+===================================	C3NS   C6	16.299.1  46.150.1	1  2 8  2

PAGE 1-A

PAGE 2-A

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

AN The cobaltous amine reaction. II. Cobalt complexes of barbiturates, methimazole, methylthiouracil, naphazoline, phenytoin, sulfathiazole and 85:25322 CA TI theophylline

ΑU CS

Bult, A.
Lab. Pharm. Anal. Chem., State Univ. Groningen, Groningen, Neth.
Pharmaceutisch Weekblad (1976), 111(17), 385-93
CODEN: PHWEAW; ISSN: 0031-6911 S0

```
Journal
DT
         English
LA
         63-5 (Pharmaceuticals)
CC
         Section cross-reference(s): 64
         The complexes of the composition Cox2(amine)2(X = anion of barbital,
AB
         hexobarbital, methylphenobarbital, pentobarbital, phenobarbital, theophylline, and sulfathiazole; amine = isobutylamine, isopropylamine or
        theophylline, and sulfathiazole; amine = isobutylamine, isopropylamine or NH3) are pseudo tetrahedral (Co(II) complexes. Co(II) coordinates with the barbiturates via N-I, with theophylline via N-7 or N-9, with sulfathiazole via the tertiary N atom of the thiazole ring. With X = anion of phenytoin the octahedral complex Co(II)x2(amine)4 is formed. This pink complex dissolves CHCl3 to a violet tetrahedral complex. With a large excess of amine the tetrahedral is converted to an octahedral. The donor atom in X is N-3. With X = naphazoline the (pseudo) tetrahedral Co(II) complexes CoX2(acetate)2 and [CoX4](Clo4)2 are prepared The pos. charge of Co2+ is compensated by acetate (coordinated) and Clo4-(uncoordinated resp. The donor atom in X is the tertiary Atom. With use of the ir spectra of previously described Co(II) complexes of methimazole a contribution to the interpretation of the ir spectrum of this drug is given. With X = anion of methylthiouracil some Co(III) complexes with the average composition CoX2(amine)n (n = .apprx.3) are prepared The lable data
available data
          are insufficient for assigning the structure.
          cobalt drug complex structure
ST
          Pharmaceuticals
IT
                (complexes with cobalt, preparation and mol. structure of)
         Molecular structure
IT
                (of cobalt-pharmaceutical complexes)
                                                                                          59653-28-0P
                                                                                                                     59680-97-6P
                                                               59448-20-3P
          59448-18-9P
                                     59448-19-0P
IT
                                                                                                                     59710-37-1P
                                                                                          59710-35-9P
                                                               59710-34-8P
          59681-00-4P
                                     59710-33-7P
                                    59710-40-6P
                                                               59710-41-7P
          59710-39-3P
          RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
                (preparation and mol. structure of)
          ANSWER 105 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
          57286-71-2 REGISTRY
RN
          Entered STN: 16 Nov 1984
Copper, bis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
ED
CN
OTHER CA INDEX NAMES:
          1-Butanamine, copper complex
CN
          C10 H22 Cu N4 S2
MF
CI
          CCS
                                  CA, CAPLUS
          STN Files:
LC
                                                         Journal
DT.CA CAplus document type:
RL.NP Roles from non-patents: PREP (Preparation)
                     NH2-Bu-n
                             1 REFERENCES IN FILE CA (1907 TO DATE)
                             1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
```

AN

TI

83:187668

CA

Copper(II) aminothiocyanates and aminoselenocyanates

```
Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V. Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
ΑU
CS
SO
        CODEN: UKZHAU; ISSN: 0041-6045
        Journal
DT
        Russian
LA
        78-7 (Inorganic Chemicals and Reactions)
        Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2, RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy = 2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes
CC
AB
        except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded. The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are
        copper amine selenocyanate thiocyanate; bipyridine copper
ST
        pseudohalogenide; phénanthroline copper pseudohalogenide
19319-87-0P 22937-31-1P 25370-74-5P 57286-42-7P
                                                                                                        57286-44-9P
                                                        253/U-/4-5P 5/286-42-7P 57286-71-2P
IT
                                                                                                       57286-73-4P
                                57286-69-8P
        57286-68-7P
        RL: SPN (Synthetic preparation); PREP (Preparation)
              (preparation of)
        ANSWER 106 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        57286-70-1 REGISTRY
RN
        Entered STN: 16 Nov 1984
ED
        Copper, bis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
        1-Propanamine, copper complex C8 H18 Cu N4 S2
CN
MF
        CCS
CI
        STN Files:
                              CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
                  NH2-Pr-n
S== C== N= C== S
                  NH2-Pr-n
                          1 REFERENCES IN FILE CA (1907 TO DATE)
                         1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
AN
        Copper(II) aminothiocyanates and aminoselenocyanates savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V. Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
        83:187668 CA
TI
ΑU
CS
SO
         CODEN: UKZHAU; ISSN: 0041-6045
DT
         Journal
LA
        78-7 (Inorganic Chemicals and Reactions)
Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2,
RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy =
2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and
Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes
         Russian
CC
AB
         except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded.
```

```
The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these
     complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are
     N-bonded.
     copper amine selenocyanate thiocyanate; bipyridine copper
ST
     pseudohalogenide; phénanthroline copper pseudohalogenide
                                                                       57286-44-9P
                                                      57286-42-7P
                                    25370-74-5P
                     22937-31-1P
     19319-87-0P
IT
                                                      57286-71-2P
                                                                       57286-73-4P
                                      57286-70-1P
                      57286-69-8P
     57286-68-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     ANSWER 107 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN 57286-68-7 REGISTRY
L9
RN
     Entered STN: 16 Nov 1984
ED
     Copper, bis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
CN
     C4 H10 Cu N4 S2
MF
     CCS
CI
     STN Files:
                    CA, CAPLUS
       CAplus document type: Journal
DT.CA
       Roles from non-patents: PREP (Preparation)
        Me-NH2
                 - N== C== S
           - Cu-
        Me-NH2
                 2 REFERENCES IN FILE CA (1907 TO DATE)
                 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
AN
     Interaction of copper powder with nonaqueous solutions of methylammonium
TI
      Babich, O. A.; Kokozei, V. N.; Pavlenko, V. A.
ΑU
      Kiev. Gos. Univ., Kiev, Ukraine
CS
      Zhurnal Neorganicheskoi Khimii (1996), 41(1), 79-82
SO
      CODEN: ZNOKAQ; ISSN: 0044-457X
     MAIK Nauka
PB
DT
      Journal
      Russian
LA
      78-7 (Inorganic Chemicals and Reactions)
CC
      Section cross-reference(s): 75
     The interaction of Cu powder with MeCN, MeOH, DMSO, and DMF solns. of
AB
     methylammonium bromide, iodide, or thiocyanate was studied. Products of the interaction were isolated and identified. The crystalline structure of [Cu(CH3NH2)4]I2 was detd (monoclinic, P21/n, a = 7.088(1), b = 8.872(1), c
     = 10.590(1) Å, β = 95.29(1)°, V = 663.04 Å3, Z = 2, ρc = 2.212 g/cm3, μ(CuKα) = 390.3 cm-1, F(000) = 414, T = 20°, 1043 reflections with I > 3σ(I), R = 0.061, RW = 0.090).
      copper reaction methylammonium salt nonaq solvent; crystal structure
ST
      copper methylamine iodide
      Crystal structure
IT
      Molecular structure
         (of tetrakis(methylamine)copper(II) iodide)
      177604-59-0P
IT
      RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
         (preparation and crystal structure of)
      67-68-5DP, DMSO, copper thiocyanate methylamine complex
IT
```

```
Methylamine, copper_DMSO thiocyanato_complex_ 463-56-9DP, Thiocyanic acid
                                                          7440-50-8DP, Copper, DMSO thiocyanato
177604-57-8P 177604-58-9P
       , copper DMSO methylamine complex
      57286-68-7P
       methylamine complex
IT
IT
       Methylammonium thiocyanate
       RL: RCT (Reactant); RACT (Reactant or reagent)
           (reaction of Cu with nonaq. solns. of methylammonium salts)
REFERENCE 2
       83:187668 CA
AN
       Copper(II) aminothiocyanates and aminoselenocyanates
TI
       Savitskii, V. N.; Skopenko, V. V.; Zhumabaev, A. Zh.; Trachevskii, V. V. Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1975), 41(9), 903-8
ΑU
CS
SO
       CODEN: UKZHAU; ISSN: 0041-6045
       Journal
DT
       Russian
78-7 (Inorganic Chemicals and Reactions)
LA
      /8-/ (Inorganic Chemicals and Reactions)
Cu(RNH2)2(NCX)2 (R = Me, Pr, Bu; X = S, Se) were prepared from Cu(NO3)2,
RNH2, and KXCN in aqueous solution at 0°. Cu(bipy)(NCX)2 (bipy =
2,2'-bipyridine), Cu(phen)(NCX)2 (phen = 1,10-phenanthroline), and
Cu(bipy)2(NCX)2 were also prepared The ir data indicate that the complexes
except Cu(bipy)2(NCX)2 are isostructural and the NCX groups are N-bonded.
The elec. conductivity of Cu(bipy)2(NCX)2 indicate 1:1 electrolytes and these
complexes can be formulated as [Cu(bipy)2NCX]NCX in which NCX- groups are
CC
       N-bonded.
       copper amine selenocyanate thiocyanate; bipyridine copper
ST
       pseudohalogenide; phenanthroline copper pseudohalogenide
19319-87-0P 22937-31-1P 25370-74-5P 57286-42-7P
                                                                                        57286-44-9P
IT
                                                                    57286-71-2P
                                                                                        57286-73-4P
                                                57286-70-1P
                           57286-69-8P
       57286-68-7P
       RL: SPN (Synthetic preparation); PREP (Preparation)
            (preparation of)
       ANSWER 108 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
       54439-01-9 REGISTRY
RN
       Entered STN: 16 Nov 1984
ED
       Nickel, tetrakis(1-butanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
       1-Butanamine, nickel complex
CN
MF
       C18 H44 N6 Ni S2
CI
       STN Files:
                        CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
```

#### REFERENCE 1

```
82:38050 CA
      Nickel aminothiocyanates and aminoselenocyanates
skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A.
Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32
AN
TI
ΑU
CS
       CODEN: UKZHAU; ISSN: 0041-6045
       Journal
DT
       Russian
LA
       78-7 (Inorganic Chemicals and Reactions)
CC
       Amines in MeOH were added to MeOH-solns. containing KSCN or KSeCN and
AB
       Ni(NO3)2.6-H20 to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and
       NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral
       with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined selenocyanate nickel amine; nickel amine selenocyanate thiocyanate 54438-96-9P 54438-97-0P 54438-98-1P 54438-99-2P 54439-00-8P
ST
IT
                                                54495-94-2P
       54439-01-9P
                           54439-03-1P
       RL: SPN (Synthetic preparation); PREP (Preparation)
            (preparation of)
       ANSWER 109 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
       54438-99-2 REGISTRY
RN
       Entered STN: 16 Nov 1984
ED
       Nickel, tetrakis(1-propanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME)
CN
       C14 H36 N6 Ni S2
MF
       CCS
CI
                          CA, CAPLUS
       STN Files:
LC
DT.CA CAplus document type: Journal
          Roles from non-patents: PREP (Preparation)
```

$$\begin{array}{c|c}
 & -Pr-NH2 & -NH2-Pr-n \\
 & & NH2-Pr-n \\
 & & NH2-Pr-n \\
 & & NH2-Pr-n \\
 & & -NH2-Pr-n \\
 & -NH2-Pr-n$$

# REFERENCE 1

82:38050 CA AN Nickel aminothiocyanates and aminoselenocyanates Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A. Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimickii Zhurnal (Russian Edition) (1974), 40(11), 1129-32 TI ΑU CS S0 CODEN: UKZHAU; ISSN: 0041-6045 Journal DT Russian LA 78-7 (Inorganic Chemicals and Reactions) CC Amines in MeOH were added to MeOH solns. containing KSCN or KSeCN and AB Ni(NO3)2.6-H2O to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral with bonding of the NCS- and NCSe- ligands through the N atom. The ideata indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined selenocyanate nickel amine; nickel amine selenocyanate thiocyanate 54438-96-9P 54438-97-0P 54438-98-1P 54438-99-2P 54439-00-8P ST IT 54495-94-2P 54439-03-1P 54439-01-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) ANSWER 110 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN L9 54438-97-0 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, tetrakis(methanamine)bis(thiocyanato-N)- (9CI) (CA INDEX NAME) CN C6 H20 N6 Ni S2 MF CICCS CA, CAPLUS STN Files: LC DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PREP (Preparation)

Me- NH<sub>2</sub> NH<sub>2</sub>-Me

Me- NH<sub>2</sub> Ni 
$$\frac{2+}{N}$$
 C S

Me- NH<sub>2</sub> N  $\frac{-}{N}$  C S

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

### REFERENCE 1

82:38050 CA AN Nickel aminothiocyanates and aminoselenocyanates TI Skopenko, V. V.; Savitskii, V. N.; Stakhov, D. A. ΑU Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1974), 40(11), 1129-32 CS 50 CODEN: UKZHAU; ISSN: 0041-6045 Journal DT Russian LA 78-7 (Inorganic Chemicals and Reactions) CC Amines in MeOH were added to MeOH solns. containing KSCN or KSeCN and AB Ni(NO3)2.6-H20 to give Ni(RNH2)4(NCX)2 (R = Me, Pr, Bu; X = S, Se) and

```
NiL(NCX)2 (L = tetraethylenepentamine). These complexes are octahedral
       with bonding of the NCS- and NCSe- ligands through the N atom. The ir data indicate that only 1 NCS- and NCSe- ligand is coordinated in [NiL(NCX)]NCX. The magnetic moments of the complexes were determined selenocyanate nickel amine; nickel amine selenocyanate thiocyanate 54438-96-9P 54438-97-0P 54438-98-1P 54438-99-2P 54439-00-8P 54439-01-9P 54439-03-1P 54495-94-2P
ST
IT
        RL: SPN (Synthetic preparation); PREP (Preparation)
             (preparation of)
        ANSWER 111 OF 121. REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        53396-13-7 REGISTRY
RN
        Entered STN: 16 Nov 1984
ED
        Zinc, bis(1-butanamine)bis(methanesulfonato-0)-, (T-4)- (9CI) (CA INDEX
CN
        NAME)
OTHER CA INDEX NAMES:
        1-Butanamine, zinc complex
OTHER NAMES:
        Bis(butylamine)bis(methanesulfonato)zinc
        C10 H28 N2 O6 S2 Zn
MF
CI
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
```

#### REFERENCE 1

81:130234 CA AN Chemistry of substituted sulfuric acids. VIII. Methanesulfonates of tin(II), tin(IV), and zinc(II)
Paul, Ram C.; Kapila, V. P.; Sharma, S. K.
Dep. Chem., Panjab Univ., Chandigarh, India TI ΑU CS Indian Journal of Chemistry (1974), 12(6), 651-2 CODEN: IJOCAP; ISSN: 0019-5103 SO Journal DT English LA 78-5 (Inorganic Chemicals and Reactions) snc12(MeSO3)2, sn(MeSO3)2, and Zn(MeSO3)2 were prepared by reacting the CC AΒ resp. metal chlorides with MeSO3H. Their 1:2 adducts with pyridine and BUNH2 were prepared and their conductances studied in MeSO3H. The presence of phases Cs2M(MeSO3)4 (M = Sn or Zn) was indicated by f.p. detns. of the M(MeSO3)2-CsMeSO3 systems. methanesulfonate tin zinc; pyridine tin zinc methanesulfonate; butylamine ST tin zinc methanesulfonate 53396-10-4P 53396-11-5P 53396-09-1P 33684-80-9P 53396-08-0P IT 53408-94-9P 53408-93-8P 53396-13-7P 53396-12-6P

```
RL: SPN (Synthetic preparation); PREP (Preparation)
         (preparation of)
     ANSWER 112 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
     38441-98-4 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Cadmium, bis(1-propanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX
CN
OTHER CA INDEX NAMES:
     1-Propanamine, cadmium complex
     Cadmium, bis(isothiocyanato)bis(propylamine)-
     C8 H18 Cd N4 S2
MF
     CCS
CI
     STN Files:
                    CA, CAPLUS
LC
DT.CA CAplus document type: Journal RL.NP Roles from non-patents: PRP (Properties)
            NH2-Pr-n
                 1 REFERENCES IN FILE CA (1907 TO DATE)
                 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
AN
      77:120272 CA
     Cadmium aminothiocyanates and aminoselenocyanates
TI
     Skopenko, V. V.; Galitskaya, S. M.
ΑU
     Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
CS
SO
      CODEN: UKZHAU; ISSN: 0041-6045
      Journal
DT
LA
      Russian
     73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance,
CC
      and Other Optical Properties)
     Section cross-reference(s): 78
     The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu,
ΑB
     do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to
      the Cd atom via the N atom.
     IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
ST
     Molecular structure-property relationship (ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate
TT
         complexes)
      Infrared spectra
IT
         (of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
                                                 38255-52-6 38255-53-7
      38255-49-1
                    38255-50-4
                                   38255-51-5
IT
                                   38441-98-4
                    38271-02-2
      38255-54-8
      RL: PRP (Properties)
         (ir spectrum of, structure in relation to)
     ANSWER 113 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
Ļ9
      38255-54-8 REGISTRY
RN
      Entered STN: 16 Nov 1984
ED
      Cadmium, bis(1-butanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX
CN
```

```
NAME)
OTHER CA INDEX NAMES:
      1-Butanamine, cadmium complex
OTHER NAMES:
      Cadmium, bis(butylamine)bis(isothiocyanato)-
      C10 H22 Cd N4 S2
MF
CI
      CCS
      STN Files:
                     CA, CAPLUS
LC
DT.CA CAplus document type:
                                     Journal
RL.NP Roles from non-patents: PRP (Properties)
             NH2-Bu-n
             2+
S = C = N - Cd^{2+} N = C = S
             NH2-Bu-n
                  2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      107:184014 CA
AN
      study of the bond strength in complex compounds by proton NMR
TI
      Galitskaya, S. M.; Pavlenko, L. I.
ΑU
CS
      Vestnik L'vovskogo Politekhnicheskogo Instituta (1986), 201, 24-6
SO
      CODEN: VLPIAZ; IŠSN: 0460-0436
      Journal
DT
      Russian
LA
      65-5 (General Physical Chemistry)
CC
      Section cross-reference(s): 77
      Bond strength in MA2L2 complexes, where M = Zn, Cd, Hg; A = BuNH2; L = CN, NCS, NCSe, was studied by NMR spectra. The M-A bond strength decreases in he order Zn > Cd > Hg. In Cd complexes, the Cd-A bond strength decreases
AB
      in the order CN > NCŠ # NCSe.
      bond energy complex NMR; zinc butylamine cyano complex bond energy;
ST
      thiocyanato butylamine cadmium complex bond energy; selenocyanato butylamine cadmium complex bond energy; cadmium butylamine cyano complex
      bond energy; mercury butylamine cyano complex bond energy
      Bond energy
IT
          (in Group IIB metal complexes, NMR in study of)
      Nuclear magnetic resonance
IT
          (of Group IIB metal complexes)
                      32491-84-2 32491-88-6... 38255-54-8 38271-02-2
      32491-81-9
IT
                                         110946-25-3
                                                         110987-94-5
                       110946-24-2
      110945-33-0
      RL: PRP (Properties)
          (bond energy in, NMR in study of)
REFERENCE 2
      77:120272 CA
AN
      Cadmium aminothiocyanates and aminoselenocyanates
TI
      Skopenko, V. V.; Galitskaya, S. M.
Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
ΑU
CS
S0
      CODEN: UKZHAU; ISSN: 0041-6045
DT
      Journal
      Russian
LA
```

```
73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance,
CC
     and Other Optical Properties)
     Section cross-reference(s): 78
     The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu,
ΑB
     do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to
     the Cd atom via the N atom.

IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
ST
     Molecular structure-property relationship
         (ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate
IT
         complexes)
     Infrared spectra
IT
         (of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
                                   38255-51-5
                                                  38255-52-6
                                                                 38255-53-7
      38255-49-1
                    38255-50-4
IT
                                   38441-98-4
                    38271-02-2
     38255-54-8
     RL: PRP (Properties)
         (ir spectrum of, structure in relation to)
     ANSWER 114 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     38255-51-5 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Cadmium, bis(ethanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX NAME)
CN
OTHER CA INDEX NAMES:
     Ethanamine, cadmium complex
CN
OTHER NAMES:
      Cadmium, bis(ethylamine)bis(isothiocyanato)-
CN
     C6 H14 Cd N4 S2
MF
     CCS
CI
     STN Files:
                    CA, CAPLUS
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PRP (Properties)
               NH2-Et
                 1 REFERENCES IN FILE CA (1907 TO DATE)
                 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      77:120272 CA
AN
      Cadmium aminothiocyanates and aminoselenocyanates.
TI
     Skopenko, V. V.; Galitskaya, S. M.
Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
ΑU
CS
SO
      CODEN: UKZHAU; ISSN: 0041-6045
      Journal
DT
      Russian
LA
      73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
CC
      Section cross-reference(s): 78
The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu,
AB
      do not show evidence for the presence of bridging X groups and so
      presumably have a tetrahedral structure. The X groups are coordinated to
      the Cd atom via the N atom.
      IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
ST
```

```
Molecular structure-property relationship
IT
         (ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate
         complexes)
     Infrared spectra
IT
         (of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes) 55-49-1 38255-50-4 38255-51-5 38255-52-6 38255-53-7
     38255-49-1
IT
                                    38441-98-4
     38255-54-8
                    38271-02-2
     RL: PRP (Properties)
         (ir spectrum of, structure in relation to)
     ANSWER 115 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     38255-49-1 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Cadmium, bis(methanamine)bis(thiocyanato-N)-, (T-4)- (9CI) (CA INDEX
CN
     NAME)
OTHER NAMES:
     Cadmium, bis(isothiocyanato)bis(methylamine)-
CN
     C4 H10 Cd N4 S2
MF
CI
     CCS
     STN Files:
                    CA, CAPLUS
LC
DT.CA CAplus document type: Journal
       Roles from non-patents: PRP (Properties)
        Me-NH2
             2+
s== c== N= cd-
                 - N== C== S
        Me-NH2
                 1 REFERENCES IN FILE CA (1907 TO DATE)
                 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
      77:120272 CA
AN
      Cadmium aminothiocyanates and aminoselenocyanates
TI
     Skopenko, V. V.; Galitskaya, S. M.
Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1972), 38(7), 709-11
ΑU
CS
S0
      CODEN: UKZHAU; ISSN: 0041-6045
      Journal
DT
      Russian
I A
     73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance,
CC
      and Other Optical Properties)
     Section cross-reference(s): 78 The ir spectra of Cd(RNH2)2X2, X = NCS and NCSe, R = Me, Et, Pr, and Bu,
AB
     do not show evidence for the presence of bridging X groups and so presumably have a tetrahedral structure. The X groups are coordinated to
      the Cd atom via the N atom.
     IR cadmium alkylamine isothiocyanate; selenocyanate cadmium alkylamine IR
ST
      Molecular structure-property relationship
IT
         (ir spectra, of cadmium alkylamine isothiocyanate and isoselenocyanate complexes)
      Infrared spectra
IT
         (of cadmium alkyl amine isothiocyanate and isoselenocyanate complexes)
                                    38255-51-5
                                                   38255-52-6
                                                                 38255-53-7
                     38255-50-4
      38255-49-1
IT
                     38271-02-2
                                    38441-98-4
      38255-54-8
      RL: PRP (Properties)
         (ir spectrum of, structure in relation to)
```

```
ANSWER 116 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     36741-31-8 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
    Cobalt, tris(methanamine)bis(nitrito-N)(thiocyanato-N)- (9CI) (CA INDEX
CN
     C4 H15 Co N6 O4 S
MF
CI
     CCS
                CA, CAPLUS
     STN Files:
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)
```

```
REFERENCE 1
       77:42560 CA
AN
       Nitro methylamine complexes of cobalt(III)
       Ganiev, A. G.; Tukhtaev, Sh. Sh.; Ikramov, Kh. U.
ΑU
       Inst. Yad. Fiz., Kiev, USSR
Zhurnal Neorganicheskoi Khimii (1972), 17(5), 1384-7
CS
S0
       CODEN: ZNOKAQ; ISSN: 0044-457X Journal
DT
LA
      78-7 (Inorganic Chemicals and Reactions)
MeNH2 reacts with [Co(NO2)6]3- to give mixed complexes.
K[Co(MeNH2)2(NO2)4], (CN3H5)H[Co(MeNH2)2(NO2)4], [Co(MeNH2)3(NO2)3],
[Co(MeNH2)3(NO2)2(NCS)], [Co(MeNH2)2(NH3)(NO2)3],
[Co(MeNH2)4(NO2)2][Co(NH3)2(NO2)4] were prepared The complexes of MeNH2 are less stable than the analogous NH3 complexes.

Cohalt methylamine nitro complex: ammine cohalt
       Russian
CC
AB
       cobalt methylamine nitro complex; ammine cobalt
ST
       Ammines
IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
            (cobalt)
                                                                                       36741-34-1P
                                                                   36741-33-0P
       19589-02-7P
                           36741-31-8P
                                               36741-32-9P
IT
       36814-38-7P
       RL: SPN (Synthetic preparation); PREP (Preparation)
           (preparation of)
       ANSWER 117 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
       34406-41-2 REGISTRY
RN
       Entered STN: 16 Nov 1984
ED
       Nickel, tetrakis(butylamine)bis(dihydrogen phosphorodithioato)-,
       0,0,0,0-tetraethyl ester (8CI) (CA INDEX NAME)
       C24 H64 N4 Ni O4 P2 S4
MF
CI
       CCS
       STN Files: CA, CAPLUS
LC
```

DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: FORM (Formation, nonpreparative); PRP
(Properties)

OEt

1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

# REFERENCE 1

75:144420 CA ΑN Stepwise adduct formation of bis(0,0'-diethyldithiophosphato)nickel(II) TI with primary and secondary amines Ciullo, G.; Furlani, C.; Sestili, L.; Sgamellotti, A. ΑU Inst. Gen. Inorg. Chem., Univ. Pérugia, Perugia, Italy Inorganica Chimica Acta (1971), 5(3), 489-92 CS SO CODEN: ICHAA3; ISSN: 0020-1693 DT Journal LA English 68 (Phase Equilibriums, Chemical Equilibriums, and Solutions)
Bis(0,0'-diethyldithiophosphato)nickel(II) behaves in a qual. similar way CC AB with both primary and secondary amines in that 1:1 and 1:2 adducts are found. Data obtained for butylamine and diethylamine indicate that the difference in behavior towards primary and secondary amines is only quant., formation consts. being much smaller with the latter. Very high concn of primary amines leads also to the formation of complexes containing the chromophore (Nis2N4), presumably with monodentate dithiophosphate ligands. nickel diethyldithiophosphate complex ST Phosphorodithioic acid, 0,0-diethyl ester, nickel complexes RL: PRP (Properties); FORM (Formation, nonpreparative) (formation consts. of) IT 109-89-7D, Diethylamine, nickel 109-73-9D, Butylamine, nickel complexes IT 29970-81-8 34406-41-2 complexes RL: PRP (Properties); FORM (Formation, nonpreparative) (formation consts. of) ANSWER 118 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN ٤9 28067-98-3 REGISTRY RN Entered STN: 16 Nov 1984 ED Nickel, tetrakis(isopropylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME) C14 H36 N6 Ni S2 CN MF CICCS STN Files: CA, CAPLUS LC

DT.CA CAplus document type: Journal RL.NP Roles from non-patents: USES (Uses)

```
i-Pr-NH2 | NH2-Pr-i |
```

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

## REFERENCE 1

```
72:91917 CA
AN
        Separation of aromatic hydrocarbons using metal-organic complexes
TI
        Csikos, Rezso; Farkas, Peter
ΑU
        Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10, 107-16
CS
SO
        CODEN: MAFKAJ; ISSN: 0506-807X
        Journal
DT
        Hungarian
51 (Petroleum, Petroleum Derivatives, and Related Products)
Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their selectivity, and stability were examined arom aliph hydrocarbons clathrate senn; aliph arom hydrocarbons clathrate
        Hungarian
LA
CC
AB
        arom aliph hydrocarbons clathrate sepn; aliph arom hydrocarbons clathrate
ST
        sepn; hydrocarbons arom aliph clathrate sepn
        Nickel cyanide (Ni(CN)2), compound with ethylamine (1:1)
IT
        RL: USES (Uses)
              (in benzene derivative separation from heptane)
        62-53-3D, Aniline, nickel complexes 75-04-7D, Ethylamine, nickel complexes 75-31-0D, Isopropylamine, nickel complexes 107-10-8D
IT
        Propylamine, nickel complexes 108-89-4D, 4-Picoline, nickel complexes 108-99-6D, 3-Picoline, nickel complexes 618-36-0D, Benzylamine, \alpha-methyl-, nickel complexes 7004-58-2 14354-71-3 14875-85-5 26997-00-2 27256-97-9 27257-00-7, Ethylamine, compound with nickel
                                                  27257-00-7, Ethylamine, compound with nickel 27279-99-8 27910-87-8 27910-88-9
        cyanide (Ni(CN)2) (1:1)
28067-98-3 28067-99-4
                                                    28631-77-8D, Pyridine, ethyl-, nickel complexes
        RL: USES (Uses)
              (in benzene derivative separation from heptane)
         142-82-5, uses and miscellaneous
IT
        RL: USES (Uses)
              (separation of, from benzene derivs. by amine nickel complex)
IT
         71-43-2P, preparation
         RL: PREP (Preparation)
        (separation of, from heptane by amine nickel complex) 95-47-6 106-42-3, preparation 108-38-3, preparation
IT
         RL: PROC (Process)
              (separation of, from heptane-xylene mixture by amine nickel complex)
```

```
ANSWER 119 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
        27910-88-9 REGISTRY
RN
        Entered STN: 16 Nov 1984
ED
        Nickel, tetrakis(propylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)
CN
        C14 H36 N6 Ni S2
MF
CI
        CCS
                             CA, CAPLUS
        STN Files:
LC
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
                 NH2-Pr-n
                        1 REFERENCES IN FILE CA (1907 TO DATE)
                        1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
        72:91917 CA
AN
        Separation of aromatic hydrocarbons using metal-organic complexes
ΤI
        Csikos, Rezso; Farkas, Peter
ΑU
CS
        Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10,
SO
        107-16
        CODEN: MAFKAJ; ISSN: 0506-807X
        Journal
DT
        Hungarian
LA
        51 (Petroleum, Petroleum Derivatives, and Related Products)
Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried
CC
AB
        out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu, C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and [Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine and PhNH2. Clathrate-forming ability of these complexes, their
        selectivity, and stability were examined arom aliph hydrocarbons clathrate sepn; aliph arom hydrocarbons clathrate
ST
        sepn; hydrocarbons arom aliph clathrate sepn
Nickel cyanide (Ni(CN)2), compound with ethylamine (1:1)
IT
        RL: USES (Uses)
              (in benzene derivative separation from heptane)
        62-53-3D, Aniline, nickel complexes 75-04-7D, Ethylamine, nickel complexes 75-31-0D, Isopropylamine, nickel complexes 107-10-8D, Propylamine, nickel complexes 108-89-4D, 4-Picoline, nickel complexes 108-99-6D, 3-Picoline, nickel complexes 618-36-0D, Benzylamine, α-methyl-, nickel complexes 7004-58-2 14354-71-3 14875-85-5 26997-00-2 27256-97-9 27257-00-7, Ethylamine, compound with nickel complexes (Ni(CN)2) (1:1) 27270-00-8 27010-87 8 27010-88 9
IT
                                                   27257-00-7, Ethylamine, compound with nickel 27279-99-8 27910-87-8 27910-88-9
        cyanide (Ni(CN)2) (1:1) 28067-98-3 28067-99-4
                                                   28631-77-8D, Pyridine, ethyl-, nickel complexes
        RL: USES (Uses)
```

(in benzene derivative separation from heptane)

142-82-5, uses and miscellaneous

IT

```
RL: USES (Uses)
            (separation of, from benzene derivs. by amine nickel complex)
       71-43-2P, preparation RL: PREP (Preparation)
IT
            (separation of, from heptane by amine nickel complex)
17-6 106-42-3, preparation 108-38-3, preparation
       95-47-6
IT
       RL: PROC (Process)
           (separation of, from heptane-xylene mixture by amine nickel complex)
       ANSWER 120 OF 121 REGISTRY COPYRIGHT 2006 ACS ON STN
L9
       27910-87-8 REGISTRY
RN
       Entered STN: 16 Nov 1984
       Nickel, tetrakis(ethylamine)bis(thiocyanato)- (8CI) (CA INDEX NAME)
ED
CN
       C10 H28 N6 Ni S2
MF
CI
       CCS
                       CA, CAPLUS
       STN Files:
LÇ
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: USES (Uses)
            NH2-Et
                 NH2-Et
             NH2-Et
                      1 REFERENCES IN FILE CA (1907 TO DATE)
                      1 REFERENCES IN FILE CAPLUS (1907 TO DATE)
REFERENCE 1
AN
       Separation of aromatic hydrocarbons using metal-organic complexes
TI
       Csikos, Rezso; Farkas, Peter
ΑU
CS
       Magyar Asvanyolaj- es Foldgazkiserleti Intezet Kozlemenyei (1969), 10,
SO
       107-16
        CODEN: MAFKAJ; ISSN: 0506-807X
        Journal
DT
       Thungarian
51 (Petroleum, Petroleum Derivatives, and Related Products)
Separation of C6H6 and xylene isomers from aliphatic hydrocarbons were carried out using complexes such as [Ni(CN)2.RNH2], where R = Et, Pr, iso-Pr, Bu,
C5H11 and C8H17; [Ni(SCN)2(R'NH2)4], R' = Et, Pr, iso-Pr and
[Ni(SCN)2(R'')4] R'' = 4-methylpyridine, 3-methylpyridine, ethylpyridine
and PhNH2. Clathrate-forming ability of these complexes, their
LA
CC
AB
       selectivity, and stability were examined arom aliph hydrocarbons clathrate sepn; aliph arom hydrocarbons clathrate
ST
        sepn; hydrocarbons arom aliph clathrate sepn
       Nickel cyanide (Ni(CN)2), compound with ethylamine (1:1)
IT
        RL: USES (Uses)
            (in benzene derivative separation from heptane)
       62-53-3D, Aniline, nickel complexes 75-04-7D, Ethylamine, nickel complexes 75-31-0D, Isopropylamine, nickel complexes 107-10-8D, Propylamine, nickel complexes 108-89-4D, 4-Picoline, nickel complexes
IT
```

```
108-99-6D, 3-Picoline, nickel complexes
                                                     618-36-0D, Benzylamine,
     α-methyl-, nickel complexes
26997-00-2 27256-97-9 27
                                                     14354-71-3
                                                                    14875-85-5
                                       7004-58-2
                                   27257-00-7, Ethylamine, compound with nickel
                                   27279-99-8 27910-87-8 27910-88-9 28631-77-8D, Pyridine, ethyl-, nickel complexes
     cyanide (Ni(CN)2) (1:1)
     28067-98-3
                    28067-99-4
     RL: USES (Uses)
         (in benzene derivative separation from heptane)
     142-82-5, uses and miscellaneous
IT
     RL: USES (Uses)
         (separation of, from benzene derivs. by amine nickel complex)
     71-43-2P, preparation
IT
     RL: PREP (Preparation)
         (separation of, from heptane by amine nickel complex) 47-6 106-42-3, preparation 108-38-3, preparation
     95-47-6
IT
     RL: PROC (Process)
         (separation of, from heptane-xylene mixture by amine nickel complex)
     ANSWER 121 OF 121 REGISTRY COPYRIGHT 2006 ACS on STN
L9
     15214-57-0 REGISTRY
RN
     Entered STN: 16 Nov 1984
ED
     Zinc, bis(2(3H)-benzothiazolethionato-xS2)bis(2-methyl-2-
CN
     propanamine)-, (T-4)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     2(3H)-Benzothiazolethione, zinc complex
CN
     2-Propanamine, 2-methyl-, zinc complex Zinc, bis(2(3H)-benzothiazolethionato-S2)bis(2-methyl-2-propanamine)-,
CN
CN
     Zinc, bis(2-benzothiazolethiolato)bis(tert-butylamine)- (7CI)
C22 H30 N4 S4 Zn
CN
MF
     CCS
CI
     STN Files:
                    CA, CAOLD, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); USES (Uses)
Ring System Data
Elemental|Elemental| Size of |Ring System|
                                                   Ring
                                    Formula
                                               |Identifier|Occurrence
Analysis |Sequence | the Rings |
                                                   RID
                                                           | Count
                                       RF
               ES
                          SΖ
   EA
                                               |333.521.13|2
                                 1C7NS
C3NS-C6 | NCSC2-C6 | 5-6
```

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1

```
132:36842 CA
AN
       Insights into sulfur vulcanization from QSPR quantitative
TI
       structure-property relationships studies
       Ignatz-Hoover, Fred; Katritzky, Alan R.; Lobanov, Victor S.; Karelson,
ΑU
       Flexsys America LP, Akron, OH, USA
CS
      Rubber Chemistry and Technology (1999), 72(2), 318-333 CODEN: RCTEA4; ISSN: 0035-9475
SO
       American Chemical Society, Rubber Division
PB
DT
       Journal
       English
LA
       39-10 (Synthetic Elastomers and Natural Rubber)
CC
      vulcanization of styrene-butadiene rubber, as accelerated by a series of sulfenamides and sulfenimides prepared from various aromatic heterocyclic
AΒ
      thiols and various aliphatic amines, was studied using the curemeter under isothermal conditions. Further studies using MOPAC AM1 semiempirical quantum mech. calcns. and CODESSA QSAR software yielded excellent correlations of mol. descriptors of accelerators or accelerator thiolate zinc complexes to the onset of cure and maximum rate of vulcanization. The QSAR results support previously proposed mechanisms describing the origin of scorch delay for the delayed action, fast curing sulfenamide accelerators. In addition, the results support a carbanionic concerted
                           In addition, the results support a carbanionic concerted
       accelerators.
       mechanism for the sulfurization and crosslinking reactions.
       sulfur vulcanization SBR quant structure property relationship
ST
       Molecular structure-property relationship
IT
       Sulfidation
       Vulcanization
       Vulcanization accelerators and agents
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       Styrene-butadiene rubber, processes
IT
       RL: PEP (Physical, engineering or chemical process); PROC (Process) (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
                                                                  7704-34-9, sulfur, uses
                                 102-77-2
                   95-33-0
                                                  4979-32-2
       95-29-4
IT
                                                                               26773-69-3
                                           15214-57-0
                                                             15670-77-6
                         15214-44-5
       10220-34-5
                                                                               137376-19-3
                        37765-44-9
                                           38335-52-3
                                                             38818-08-5
       36930-73-1
                                                                                     252564-20-8
                                                                 188036-96-6
                                             157993-40-3
       156017-14-0
                          156477-90-6
                                                                                     252564-25-3
                                                                 252564-24-2
                                              252564-23-1
                          252564-22-0
       252564-21-9
                                                                                     252564-30-0
                                             252564-28-6
                                                                 252564-29-7
                          252564-27-5
       252564-26-4
                                                                                     252564-35-5
                                             252564-33-3
252564-38-8
                                                                 252564-34-4
       252564-31-1
                          252564-32-2
                                                                 252564-83-3
                          252564-37-7
       252564-36-6
      RL: MOA (Modifier or additive use); USES (Uses)
(insights into sulfur vulcanization from quant. structure-property relationships studies)
       95-31-8, N-tert-Butylbenzothiazole-2-sulfenamide
IT
      RL: MOA (Modifier or additive use); RCT (Reactant); RACT (Reactant or
       reagent); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
IT
       252564-18-4P
       RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP
       (Preparation); USES (Uses)
           (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
       37143-54-7, 1-Methoxy-2-propylamine
IT
       RL: RCT (Reactant); RACT (Reactant or reagent) (insights into sulfur vulcanization from quant. structure-property
           relationships studies)
IT
       9003-55-8
```

```
RL: PEP (Physical, engineering or chemical process); PROC (Process)
                (styrene-butadiene rubber, insights into sulfur vulcanization from
              quant. structure-property relationships studies)
                         THERE ARE 66 CITED REFERENCES_AVAILABLE FOR THIS RECORD
RE.CNT
(1) Anon; Natural Rubber Science and Technology 1988, P570
(2) Balaban, A; Chem Phys Lett 1982, V89, P399 CAPLUS (3) Barton, B; J Ind Eng Chem 1952, V44, P2444 CAPLUS
(4) Bateman, L; The Chemistry and Physics of Rubber-Like Substances 1963, P449
(5) Bedford, C; J Ind Eng Chem 1920, V12, P31 CAPLUS
(6) Campbell, R; Rubber Chem Technol 1964, V37, P635 CAPLUS
(7) Campbell, R; Rubber Chem Technol 1964, V37, P650 CAPLUS
(8) Chapman, A; Natural Rubber Science and Technology 1988, P511
(9) Chivers, T; Nature 1974, V252, P32 CAPLUS
(10) Coates, E; J Chem Soc 1965, P5613 CAPLUS
(11) Coran A; Rubber Chem Technol 1964, V27, P670 CAPLUS
(11) Coran, A; Rubber Chem Technol 1964, V37, P679 CAPLUS
(12) Coran, A; Rubber Chem Technol 1964, V37, P689 CAPLUS
(13) Coran, A; Rubber Chem Technol 1965, V38, P1 CAPLUS (14) Coran, A; Science and Technology of Rubber 1978, P301
(15) Coucouvanis, D; J Am Chem Soc 1967, V89, P1346 CAPLUS
(16) Ding, R; Rubber Chem Technol 1996, V69, P81 CAPLUS
(17) Fackler, J; J Am Chem Soc 1968, V90, P2784 CAPLUS
(18) Goda, K; Nippon Gomu Kyokaishi 1973, V46, P63 CAPLUS
(19) Gupta, S; J Inorg Nucl Chem 1970, V32, P1611 CAPLUS
(20) Hall, H; J Am Chem Soc 1957, V79, P5441 CAPLUS
(21) Hammett, L; Chem Rev 1935, V17, P125 CAPLUS
(22) Hann, C; Rubber Chem Technol 1994, V67, P76 CAPLUS
(23) Higgins, G; J Chem Soc 1963, P2812 CAPLUS
(24) Huibers, P; Langmuir 1996, V12, P1462 CAPLUS
(25) Karelson, M; Chem Rev 1996, V96, P1027 CAPLUS
(26) Katritzky, A; Anal Chem 1994, V66, P1799 CAPLUS
(27) Katritzky, A; CODESSA Reference Manual 1994
(28) Katritzky, A; Chem Soc Rev 1995, V24, P279 CAPLUS
(29) Katritzky, A; J Chem Inf Comput Sci 1996, V36, P879 CAPLUS
(30) Katritzky, A; J Chem Inf Comput Sci 1997, V37, P913 CAPLUS
(31) Katritzky, A; J Phys Chem 1996, V100, P10400 CAPLUS
(32) Kier, L; Molecular Connectivity in Chemistry and Drug Research 1976
(33) Kratz, G; J Ind Eng Chem 1920, V12, P317 CAPLUS
(34) Krebs, H; Rubber Chem Technol 1957, V30, P962
(35) Krejsa, M; Rubber Chem Technol 1992, V65, P427 CAPLUS
(36) Krejsa, M; Rubber Chem Technol 1994, V67, P348 CAPLUS (37) Kresja, M; Rubber Chem Technol 1993, V66, P376
 (38) Lichty, J; US 2129621 1938 CAPLUS
(39) McCleverty, J; Sulfur. Its Significance for Chemistry, for the Geo-, Bio-,
and Cosmosphere Technology 1984, V5, P31

(40) Miligan, B; Rubber Chem Technol 1966, V39, P1115

(41) Milligan, B; J Chem Soc 1966, V1, P34

(42) Mitchell, B; J Chem Inf Comput Sci 1997, V37, P538 CAPLUS

(43) Moore, C; J Chem Soc 1954, P2082 CAPLUS

(44) Morita, E; Rubber Chem Technol 1984, V57, P744 CAPLUS
 (45) Murugan, R; Chemtech 1994, V24(6), P17 CAPLUS
(46) Porter, M; Perspectives in the Organic Chemistry of Sulfur 1987, P267
       CAPLUS
 (47) Porter, M; The Chemistry of Sulfides 1977
 (48) Randic, M; J Am Chem Soc 1975, V97, P6609 CAPLUS
(49) Reid Shelton, J; Rubber Chem Technol 1960, V33, P342 (50) Rogers, D; J Chem Inf Comput Sci 1994, V34, P854 CAPLUS
(51) Rostek, C; Rubber Chem Technol 1996, V69, P180 CAPLUS (52) Skinner, T; Rubber Chem Technol 1972, V45, P182 CAPLUS (53) Spacu, G; Bull Sect Sci Acad Roum 1938-1939, V21, P173
 (54) Stanton, D; Anal Chem 1990, V62, P2323 CAPLUS
(55) Sullivan, A; Rubber Chem Technol 1992, V65, P488 CAPLUS
```

```
(56) Sutter, J; J Chem Inf Comput Sci 1995, V35, P77 CAPLUS (57) Sutter, J; J Chem Inf Comput Sci 1996, V36, P100 CAPLUS (58) Taft, R; J Am Chem Soc 1952, V74, P3120 CAPLUS (59) Taft, R; Steric Effects in Organic Chemistry 1956, P556 CAPLUS (60) Tetko, I; J Chem Inf Comput Sci 1996, V36, P794 CAPLUS (61) Tsurugi, J; J Soc Rubber Ind Jpn 1952, V25, P267 CAPLUS (62) Vander K; Pubber Chem Tochnol 1994, V67, P106
(62) Vander, K; Rubber Chem Technol 1994, V67, P196
(63) Watson, A; PhD Thesis University of London 1965, P53 (64) Wessel, M; J Chem Inf Comput Sci 1995, V35, P841 CAPLUS (65) Wiener, H; J Am Chem Soc 1947, V69, P17 CAPLUS (66) Wolfe, J; Rubber Chem Technol 1968, V41, P1339 CAPLUS
REFERENCE 2
              64:33012
ΑN
              Vulcanization accelerator-activator complexes. I. Amine complexes of zinc
TI
              and cadmium benzothiazole-2-thiolate
              Milligan, Brian
ΑU
              Nat. Rubber Producers' Res. Assoc., Welwyn Garden City, UK
              J. Chem. Soc., Inorg., Phys., Theoret. (1966), (1), 34-5
SO
              Journal
DT
              Enalish
LA
              14 (Inorganic Chemicals and Reactions)
CC
              Eleven amine complexes of Zn benzothiazole-2-thiolate were prepared from the NH3 complex. Dissociation of the pyridine complex provides a convenient route to the thiolate, which is difficult to prepare by other methods.
AB
              Rubber
IT
                        (vulcanization accelerator-activator complexes)
               Rubber
IT
                        (vulcanization accelerators for, 2-benzothiazolethiol complexes with Cd
                        and Zn as)
              Zinc, bis(2-benzothiazolethiolato)-, compound with ethylenediamine (1:3)
IT
               tert-Butylamine, zinc complex with 2-benzothiazolethiol
               RL: PREP (Preparation)
                                                                                               110-89-4, Piperidine
               108-91-8, Cyclohexylamine
IT
                        (complexes of Cd and Zn with 2-benzothiazolethiol and)
               149-30-4, 2-Benzothiazolethiol
IT
                        (complexes of Cd and Zn with amines and, rubber vulcanization
                        accelerator-activator complexes)
               149-30-4, 2-Benzothiazolethiol
IT
                        (complexes with Cd and Zn)
               97-39-2P, Guanidine, 1,3-di-o-tolyl-, zinc complex with
              9/-39-2P, Guanidine, 1,3-di-o-tolyl-, Zinc complex with 2-benzothiazolethiol 100-46-9P, Benzylamine, zinc complex with 2-benzothiazolethiol 107-15-3P, Ethylenediamine, compds. with bis(2-henzothiazolethiolato)zinc (3:1) 107-15-3P, Ethylenediamine, zinc complex with 2-benzothiazolethiol 110-86-1P, Pyridine, zinc complex with 2-benzothiazolethiol 110-91-8P, Morpholine, zinc complex with 2-benzothiazolethiol 141-43-5P, Ethanol, 2-amino-, zinc complex with 2-benzothiazolethiol 12194-64-8P, Zinc, bis(2-benzothiazolethiolato)bis(1.3-diphenvlquanidine)- 12204-85-2P. Zinc.
IT
                                                                                                                                                                      12204-85-2P, Zinc.
                benzothiazolethiolato)bis(1,3-diphenylguanidine)-
               bis(2-benzothiazolethiolato)bis(1,3-di-o-tolylguanidine)-
zinc, bis(2-benzothiazolethiolato)bis(pyridine)- 14807-7
bis(2-benzothiazolethiolato)- 15214-44-5P, Zinc, bis(2-
                                                                                                                                                                                           14740-86-4P
                                                                                                                                                                   14807-72-8P, Cadmium,
               Zinc, bis(2-benzothiazolethiolato) 15214-44-5P, Zinc, bis(2-benzothiazolethiolato) 15214-44-5P, Zinc, bis(2-benzothiazolethiolato) bis(morpholine) 15214-57-0P, Zinc, benzothiazolethiolato) bis(tert-butylamine) 15278-06-5P, Zinc, codming of the color bis (tert-butylamine) 15278-06-5P, Zinc, bis (2-benzothiazolethialato) bis (tert-butylamine) 15278-06-5P, Zinc, bis (2-benzothialato) bis (tert-butylamine) 15278-06-5P, Zinc, bis (2-benzothialato) b
               bis(2-benzothiazolethiolato)bis(tert-butylamine)-bis(2-benzothiazolethiolato)bis(2-aminoethanol)-
                                                                                                                                                                   15612-28-9P, Cadmium,
               bis(2-benzothiazolethiolato)bis(piperidine)-
bis(2-benzothiazolethiolato)bis(piperidine)-
bis(2-benzothiazolethiolato)bis(benzylamine)-
                                                                                                                                                        15627-29-9P, Zinc,
                                                                                                                                                        15669-72-4P, Zinc,
                                                                                                                                                         15670-75-4P, Cadmium,
                bis(2-benzothiazolethiolato)bis(cyclohexylamine)-
                                                                                                                                                                      15670-77-6P, Zinc,
```

bis(2-benzothiazolethiolato)bis(cyclohexylamine)- 15682-25-4P, Zinc, bis(2-benzothiazolethiolato)(ethylenediamine)- 18907-31-8P, Zinc, bis(2-benzothiazolethiolato)- RL: PREP (Preparation) (preparation of)

=> FIL STNGUIDE SINCE FILE TOTAL COST IN U.S. DOLLARS **SESSION ENTRY** 557.97 1372.33 FULL ESTIMATED COST TOTAL SINCE FILE DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) **SESSION ENTRY** -98.40-63.90CA SUBSCRIBER PRICE

FILE 'STNGUIDE' ENTERED AT 05:27:45 ON 11 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION. LAST RELOADED: Dec 8, 2006 (20061208/UP).

=> FIL CAPLUS SINCE FILE TOTAL COST IN U.S. DOLLARS **SESSION ENTRY** 1.08 1373.41 **FULL ESTIMATED COST** SINCE FILE TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) **ENTRY** SESSION -98.40 0.00 CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 05:38:32 ON 11 DEC 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 11 Dec 2006 VOL 145 ISS 25 FILE LAST UPDATED: 10 Dec 2006 (20061210/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> FIL STNGUIDE
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.46 1373.87